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Low Nox Combustion Concepts for Advanced Power Generation Systems Firing Low-Btu Gas

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LOW NO_x COMBUSTION CONCEPTS FOR ADVANCED POWER GENERATION SYSTEMS FIRING LOW-BTU GAS

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16. ABSTRACT The report gives results of an analysis of several advanced power generating concepts firing low-Btu gasified coal. A combined gas-turbine/steam-cycle power plant with integrated gasifier was the most promising from fuel utilization and economic viewpoints. Two representative combined cycle systems were chosen for detailed NOx emission and analysis: an advanced-technology high-temperature gas turbine with a waste heat boiler; and a supercharged boiler with a current-technology gas turbine. NOx emissions were investigated using a kinetic model, which was validated by comparison with best available experimental data and then applied to idealized combustor configurations. Calculations indicate that staged combustion involving rich primary zones and controlled mixing secondary zones minimizes thermal NOx and NOx produced from ammonia in the fuel gas. Minimum calculated NOx levels were: 150 ppm for the high temperature turbine, with a 0.45 equivalence ratio and 4000 ppm of fuel ammonia; and 125 ppm for the supercharged boiler, with 5% excess air and 500 ppm of fuel ammonia. These results need to be verified experimentally, but they show the potential for achieving NOx emissions within the Federal NSPS without requiring ammonia removal from the fuel gas.

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by

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SUMMARY

Several advanced power generating concepts firing low Btu gasified coal were analyzed and the combined gas and steam cycle power plant with integrated gasifier was identified as the most promising from fuel utilization and economic points of view. Two representative combined cycle systems were chosen for detailed nitrogen oxide emission analysis: (1) an advanced-technology high-temperature gas turbine with a waste heat boiler; and (2) a supercharged boiler with a current-technology gas turbine. Nitrogen oxide emissions were investigated using a kinetic model which included over 100 reactions. The model was validated by comparison with the best available experimental data and then applied to idealized combustor configurations.

Staged combustion schemes involving rich primary zones and controlled mixing secondary zones were found to minimize thermal nitrogen oxides and nitrogen oxides produced from ammonia in the fuel gas. The minimum calculated nitrogen oxide levels were 150 ppm for the high temperature turbine case with an equivalence ratio of 0.45 and 4000 ppm of fuel ammonia, and 125 ppm for the supercharged boiler with five percent excess air and 500 ppm of fuel ammonia. Both these calculations refer to uncorrected concentrations measured at the stated equivalence ratio. While these results need to be verified experimentally, they show the potential for nitrogen oxide emissions within the Federal New Source Performance Standards without requiring ammonia removal from the fuel gas.

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1.0 INTRODUCTION

Although the United States has an abundant supply of coal, the utilization of this resource has been hindered by the low competitive cost of petroleum, its availability from foreign sources and its proven technology. However, the recent rise in petroleum prices and the vulnerability of foreign supply to international politics encourage the development of domestic coal resources as a petroleum alternative.

Unfortunately, coal causes more environmental problems than petroleum. One of the most severe problems is the high sulfur content of coal and the corresponding sulfur oxide emissions. Much of the recent coal-related research has focused on this problem and several approaches have been explored: direct coal combustion with stack gas scrubbers to remove sulfur oxides, use of sorbants for sulfur oxide control in fluidized bed combustors, and the conversion of coal into low sulfur gaseous or liquid fuels. While each of these options can potentially decrease emissions of sulfur oxides to acceptable levels, the total environmental impact of each option from coal extraction to final end use must be considered. This report examines one aspect of this problem, the nitrogen oxide emissions from advanced power systems fired with low Btu gasified coal (LBG).

The primary justification for using low Btu gas (LBG) in advanced power systems is the potential for reduced sulfur emissions with improved thermodynamic performance over conventional coal-fired power plants. Technological and economic obstacles limit conventional plants without sulfur recovery to overall efficiencies (coal pile to buss bar) in the range of 37 to 40 percent. However, essentially all of the sulfur entering such plants in the form of coal exits in the stack gas in the form of SO_2. Federal New Source Performance Standards limit SO_2 emissions from coal-fired steam boilers to 1.2 pounds of SO_2 per 10^6 Btu heat release. This corresponds to 0.6 weight percent sulfur in a coal with a heating value of 10,000 Btu/lb. Compliance with this regulation requires either low sulfur coal or sulfur removal from the coal or stack gas. However, low sulfur coal is in short supply and sulfur removal or stack gas cleaning can lower overall efficiency to the low 30 percent range. These factors have motivated a search for alternate solutions which are more efficient and environmentally acceptable methods of coal utilization.

Low Btu coal gasification offers such an alternative solution. Since the gasification process operates fuel-rich, the sulfur in the coal is converted mainly to H_2S in the fuel gas which can be removed more easily than SO_2. The H_2S concentration is high and the total volume of gas to be treated is small in comparison with SO_2 scrubbing.

The production of LBG has the disadvantage that the energy losses in the gasification and sulfur cleanup processes may amount to more than 25 percent of the coal's heating value. These losses must be countered with improvements in integrated gasification and power system design if the overall energy conversion is to be economically competitive with conventional direct-fired power plants with stack gas sulfur removal. One major energy loss is the sensible heat of the hot LBG leaving the gasifier. This heat, amounting to 10 to 15 percent of the coal's heat of combustion, is lost or used inefficiently if the sulfur cleanup must be carried out at low temperatures. The use of a high temperature cleanup process offers reduced losses since the sensible heat adds to the heat released in final combustion. Modifying the plant's thermodynamic cycle is another possible improvement. Although direct coal conversion is limited by present technology to furnace firing, LBG can be combusted in internal combustion engines such as gas turbines. The hot turbine exhaust gases can also be used as a heat source for a steam cycle giving rise to a combined gas and steam (COGAS) cycle. With turbine inlet temperatures representative of current technology (2000^oF) overall COGAS plant efficiencies are comparable to conventional direct coal-fired plants without sulfur recovery. With the promise of increased turbine inlet temperatures the COGAS system can yield efficiencies significantly greater than conventional power plants.

The environmental consequences of burning LBG in advanced power generation systems are not well-known. The precise composition of LBG depends upon the coal characteristics and the details of the gasification process. The major fuel gases contain small amounts of hydrogen sulfide, carbonyl sulfide and ammonia. Although methods of sulfur removal are well-documented the fate of the ammonia is less certain. Robson, et al(1) estimate up to 600 ppm of ammonia in a low Btu gas with low temperature cleanup and 3,800 ppm from high temperature cleanup processes currently under development.

A substantial portion of the ammonia could be converted to nitric oxide in the combustion process. Previous investigations of ammonia conversion in combustion systems have shown that under premixed conditions the amount converted is dependent upon mixture stoichiometry and can be as high as 80 percent. In diffusion flames up to 50 percent of the ammonia can be converted depending on the method of ammonia addition and the rate of fuel/air mixing. Consequently, if LBG is combusted without ammonia removal the potential for nitric oxide production may be greater than in the present coal.

This report investigates the combustion of LBG in advanced power systems focusing on the rate of NO_x formation from fuel nitrogen-bearing species such as ammonia. Section 2 examines the characteristics of LBG gas. The alternative gasificiation processes, species distributions, heating value and other fuel properties are summarized. Gas cleanup systems for removing sulfur species, particulates and nitrogen-bearing species are also reviewed. The design and performance of advanced power generating systems are documented in Section 3. A comparative analysis of several alternative systems is presented and the combustion parameters for the most attractive systems are determined.

In Section 4 the rates of NO_x formation from these LBG combustion systems are estimated. A kinetic model is applied to a simplified LBG fuel containing carbon monoxide, hydrogen and methane with trace quantities of ammonia. A series of "limit-cases" are evaluated based on operating constraints imposed by practical systems. Although macro- and micro-scale mixing phenomena dictate the NO_x emission levels in any practical system, this model establishes upper and lower emission limits and thus gives an indication of the feasibility of direct use of high ammonia fuel gases.

2.0 FUEL CHARACTERISTICS

Although identified by the single term low Btu gas, the characteristics of the fuel are as varied as the air blown gasification schemes proposed for its production. This section discusses the composition of coal-derived fuel gases which could be used as fuels for power generation, their combustion characteristics and pollutant production potential. These parameters of the fuel gas depend to varying extent upon:

- the feedstock;
- the gasification process;
- the thermodynamic state of the product gas; and
- the method of product gas cleanup.

2.1 Gasification Processes

2.1.1 Gasifier Types

Low Btu Gas (LBG) is produced from coal through a partial pyrolysis reaction where coal, steam and air combine in a gasifier pressure vessel to make a hot combustible fuel gas with a heating value of approximately 150 Btu/ft^3. Three types of gasifiers have been used or proposed to be used to generate LBG:

- Fixed bed
- Fluidized bed
- Entrained Flow Gasifier

Figure 2-1 compares the characteristics of each gasifier type. The fixed bed is the oldest design and is basically a counterflow device. Air and steam are blown upward through a packed coal bed in which the reaction occurs. As the coal reacts, additional coal is continuously added at the top so that coal particles move continuously downward through four reaction zones: drying, devolatilization, gasification and char combustion. Ash is removed from the bottom. The coal bed is continuously stirred to avoid coking and temperatures are maintained low to prevent ash fusion. Typical LBG output temperatures are in the range of 800 to 1200°F. The counterflow process and the low temperature result in substantial carry-over of tars, oils and char.

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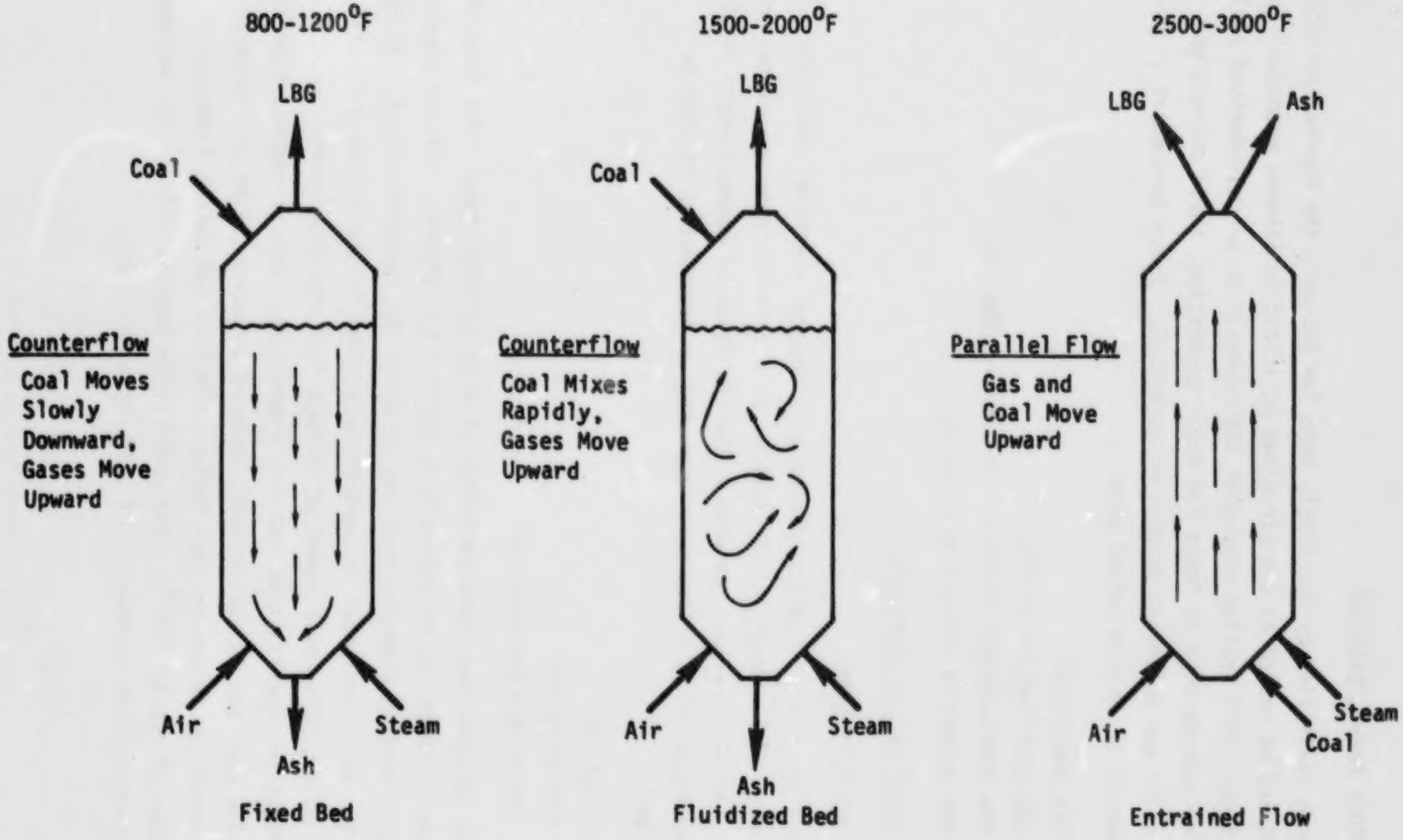
800-1200°F
LBG
Coal
Counterflow
Coal Moves Slowly Downward, Gases Move Upward
Air
Ash
Steam
Fixed Bed
1500-2000°F
LBG
Coal
Counterflow
Coal Mixes Rapidly, Gases Move Upward
Air
Ash
Steam
Fluidized Bed
2500-3000°F
LBG
Ash
Parallel Flow
Gas and Coal Move Upward
Air
Coal
Steam
Entrained Flow

Figure 2-1. Schematic Diagrams of LBG Coal Gasifiers

In fluidized bed designs the relative gas velocity is substantially higher than in fixed bed designs, and the coal bed is turbulent with substantial bottom-to-top mixing. As a first approximation the solid phase characteristics may be assumed constant from bottom to top and the four reaction zones are merged. This and the higher LBG output temperature (1500-2000°F) reduces tar and higher hydrocarbon carry-over.

Entrained flow gasifiers have the highest gas phase velocity. All components including the coal particles are introduced at the bottom and move upward. Unlike the fixed and fluidized bed gasifiers, all constituents move in essentially parallel flow. The high temperatures employed in entrained flow gasifiers (2500-3000°F) essentially eliminate higher hydrocarbons.

2.1.2 Specific Gasification Processes

Gasification processes suitable for integration into a COGAS power plant can be divided into two classes: current state-of-the-art processes which have demonstrated commercial success, and second generation processes now in the pilot plant stage. Three systems can be considered current state-of-the-art and capable of restricted present day utilization:

- Lurgi
- Koppers Totzek
- Winkler

Lurgi

The Lurgi gasifier is a pressurized, stirred, fixed bed gasifier originally developed in 1931. Figure 2-2 shows the essential design elements. Gasification takes place in a countercurrent moving bed of coal at pressures above 300 psig(3). Coal is fed intermittently through a pressurized coal lock, passes downward through the reacting bed and exits as ash through a lock hopper on the bottom.

Major operating problems center around the use of coking coals. A coal distributor rotates beneath the bed surface to prevent the coal from bonding together when it reaches the plastic state, and a rotating grate at the bottom serves the same function for ash. A water jacket surrounding the

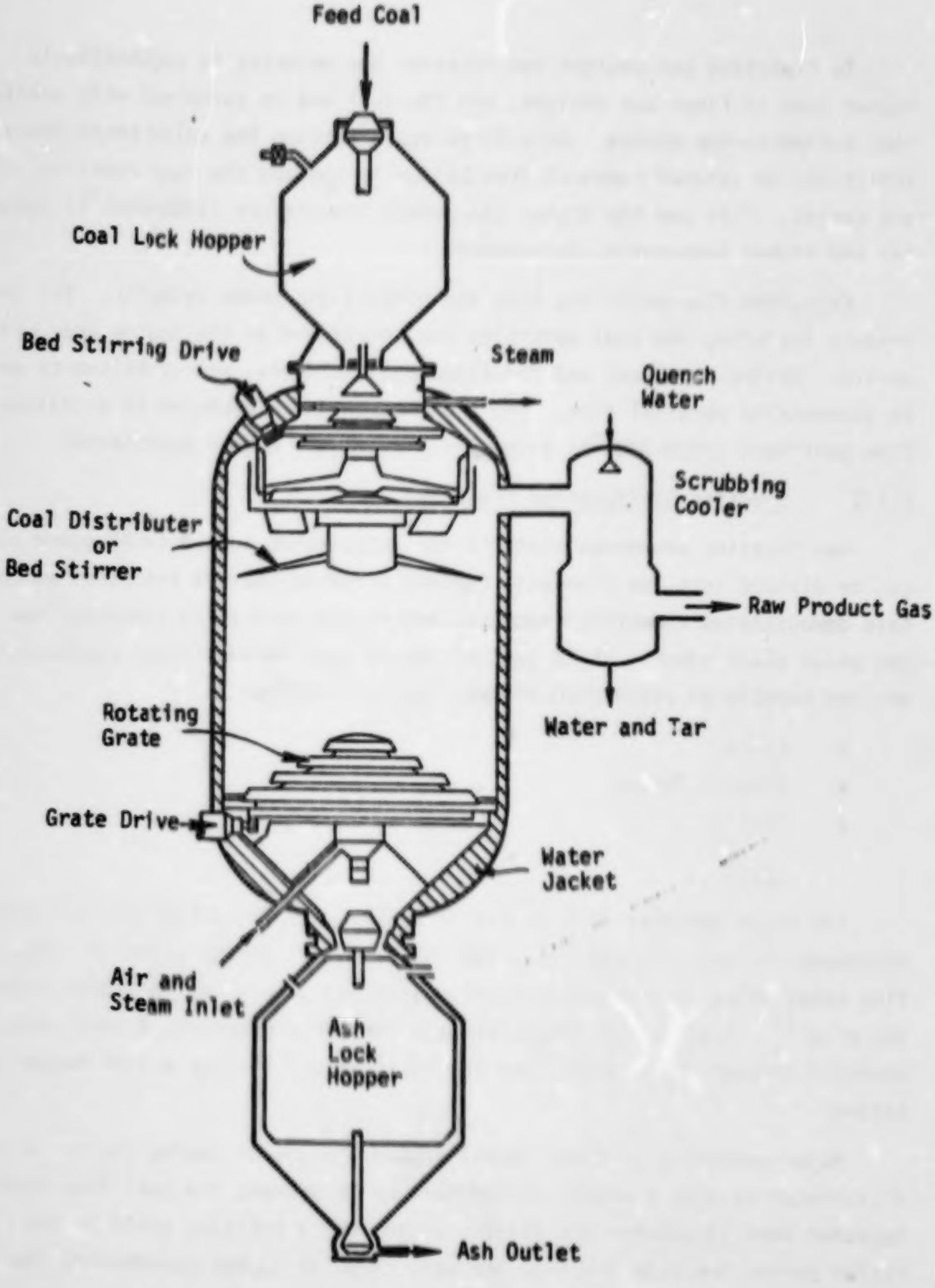
Feed Coal
Coal Lock Hopper
Bed Stirring Drive
Steam
Quench Water
Scrubbing Cooler
Coal Distributer or Bed Stirrer
Raw Product Gas
Water and Tar
Rotating Grate
Grate Drive
Water Jacket
Air and Steam Inlet
Ash Lock Hopper
Ash Outlet

Figure 2-2. Lurgi Gasifier Schematic Diagram (from Refs. 2 and 3)

gasifier vessel provides some cooling and approximately 10 percent of the steam necessary for gasification. The steam/air mixture entering the gasifier also cools the ash preventing fusion. The crude product gas leaves the gasifier between 600 and 1200°F (the temperature is a function of coal type) and contains coal dust, oil, naptha, phenol, ammonia, tar oil, ash and char, as well as CO_2, H_2, CO, CH_4, N_2, H_2S, COS and small quantities of higher hydrocarbons. The product passes through a scrubber and cooling tower to remove the tar before being cooled to about 370°F in a waste heat boiler.

The Lurgi process is complicated because of the large number of moving parts which also limits its size. Although vessels of 16 feet in diameter are planned, present day capabilities are limited to 12 feet diameter(4). The 12 feet units can produce up to 230 million Btu/hr of fuel gas and are marketed in the United States by the American Lurgi Corporation in New York.

Winkler

The Winkler generator is a fluidized bed gasifier originally developed in the 1920s for the production of synthesis gas from small friable fuels (up to 8 mm in size) which were unsuitable for gasification in fixed beds. The gasification takes place in a fluidized bed supported by steam/oxygen or steam/air - as with fixed bed gasifiers, the feed stock must be noncoking. The product gases leave the gasifier at between 1500 and 1900°F and are relatively free from condensible hydrocarbons(5). The original gasifier design operated at a pressure of 1.5 atmospheres absolute and recently the design has been reevaluated to allow high pressure operation.

The Winkler system is currently marketed by Davy Power Gas, Inc., Lakewood Florida and sizes to 18 feet diameter providing up to 500 million Btu/hr of fuel gas have been operated(4).

Koppers Totzek (K-T)

The K-T process is an entrained flow gasifier as shown in Figure 2-3. Pulverized coal, oxygen and steam are fed through a "burner" into the gasifier vessel where they react at a slight positive pressure and at approximately 3300°F(6). The ash slags and between 50-70 percent of it is removed from the water quench tank. The product gas may be water quenched before

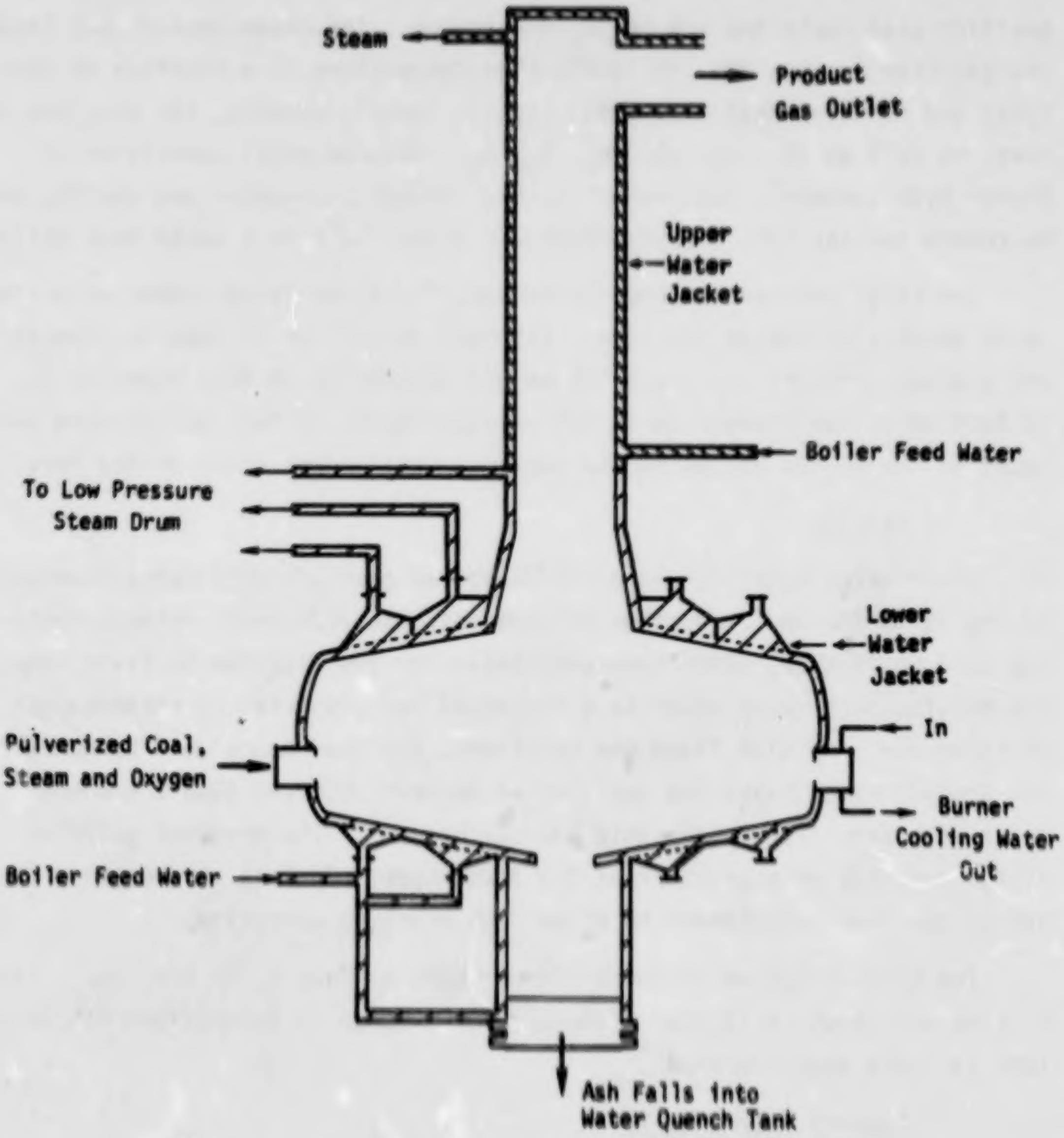
Steam
Product Gas Outlet
Upper Water Jacket
Boiler Feed Water
To Low Pressure Steam Drum
Lower Water Jacket
In
Pulverized Coal, Steam and Oxygen
Burner Cooling Water Out
Boiler Feed Water
Ash Falls into Water Quench Tank

Figure 2-3. Schematic Diagram of Koppers Totzek (K-T) Entrained Flow Gasifier

passing through a waste heat boiler and further scrubbing systems. Tests have been conducted with air instead of oxygen, but high preheat temperatures of at least 982°C must be used to maintain slagging conditions. Because of its high temperature, the K-T system is insensitive to the coal coking properties and the product gas is free of tars and other condensible hydrocarbons. However, trace amounts of NH_3 and HCN are produced.*

This system is marketed in the United States by the Koppers Co., Inc., Pittsburgh, Pennsylvania. The largests units produce up to 234 million Btu/hr and larger units up to 560 million Btu/hr are under construction(4).

The three systems described above were operable forty years ago and are not necessarily representative of future integrated coal gasifier electric power generation plants. The limitations of fixed bed gasifiers (coking and small size) will probably preclude their use in large scale COGAS plants. Similarly, unless the coking problem in fluidized bed gasifiers can be resolved, they will be limited to use with selected coal types.

Entrained flow and fluidized bed gasifiers have received increased attention in recent years since they have been recognized as suitable for large-scale LBG coal gasification(7,8). The BCR entrained flow gasifier and the Westinghouse fluidized bed gasifier are two examples of second generation gasifier systems.

Bituminous Coal Research (BCR) Entrained Flow Gasifier

Figure 2-4 is a schematic diagram of the BCR entrained flow gasifier. Gasification occurs in two stages. In the top stage crushed dried coal contacts hot gas from the lower stage and partially gasifies leaving small char and ash particles. The flow velocity is high enough to entrain the particles so that all materials exit the top of the gasifier as a gas-solid suspension. The char and slag are separated from the product gas in a cyclone separator and returned to the lower stage gasifier vessel pneumatically suspended in steam. The char reacts with the air in the lower stage and the slag drops out the bottom. Both stages operate at a nominal pressure of 500 psia and the product gas exit temperature is 1800°F(9).

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*NH_3 = 0.17 percent and HCN 288 ppm by volume(6)

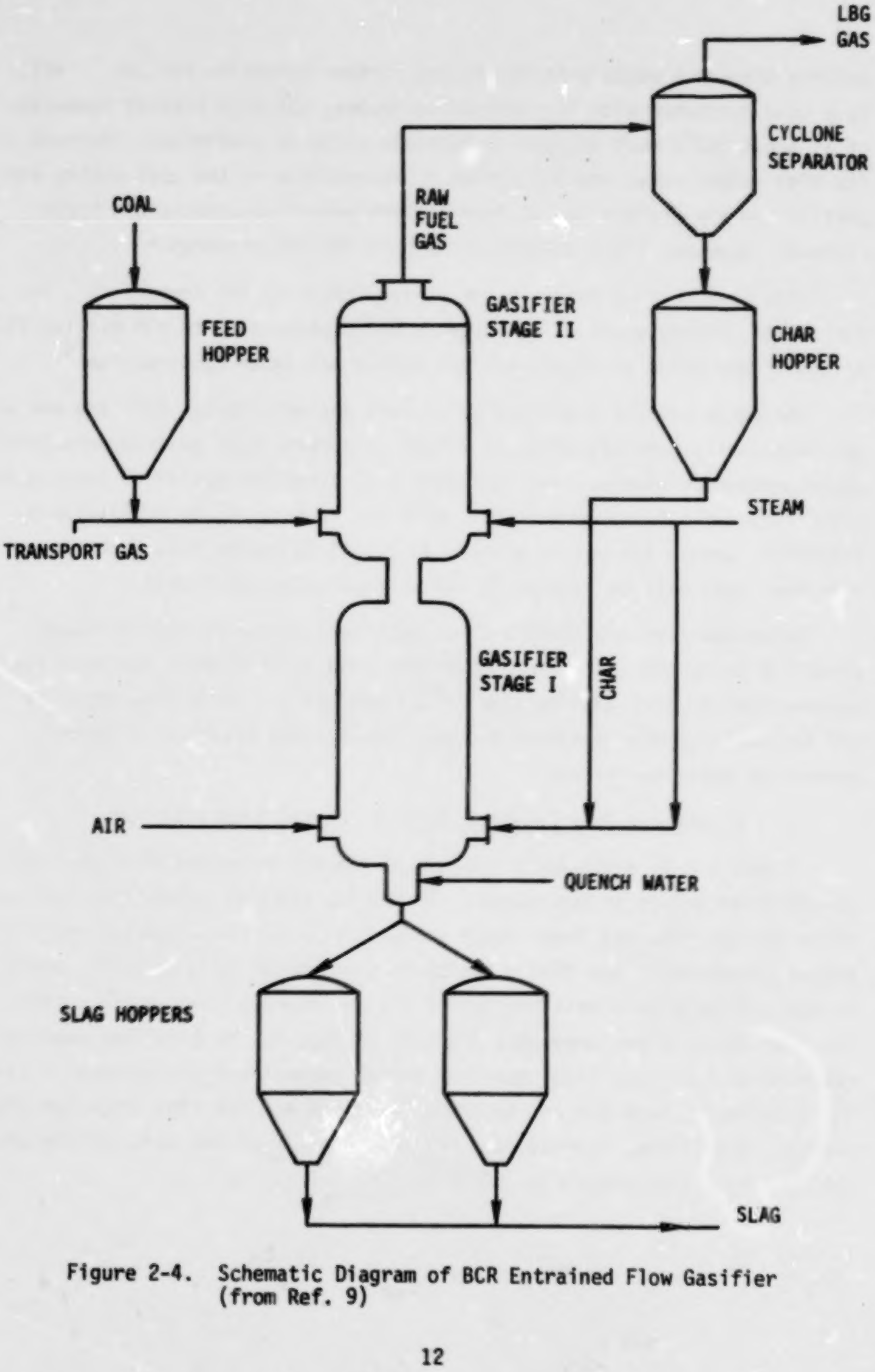
LBG
GAS
CYCLONE
SEPARATOR
RAW
FUEL
GAS
COAL
FEED
HOPPER
GASIFIER
STAGE II
CHAR
HOPPER
STEAM
TRANSPORT GAS
GASIFIER
STAGE I
CHAR
AIR
QUENCH WATER
SLAG HOPPERS
SLAG

Figure 2-4. Schematic Diagram of BCR Entrained Flow Gasifier (from Ref. 9)

Westinghouse Fluidized Bed Gasifier

The Westinghouse gasifier is a two-stage process combining sulfur removal with the gasification process as shown in Figure 2-5. The upper stage is a recirculating fluidized bed where hot coal gas and char react to form LBG, and dolomite particles absorb sulfur. Coal is introduced at the bottom, entrained at 20 to 40 ft/sec in a "draft tube" and transported to the top of the bed. Dolomite particles injected at the top move downward absorbing sulfur from the gases moving counterflow. Since char and dolomite have different densities they tend to segregate in the fluidized bed and are drawn off and rejected. Particulate-laden LBG is drawn off the top of the reactor and cleaned in a cyclone separator before exiting at $1600^{o}F$. The char is recycled to the combustor gasifier where it reacts in a fluidized bed supported by steam and air producing a hot fuel gas as a feed to the upper gasifier vessel. The Westinghouse gasifier operates at 10 to 15 atmospheres and produces LBG at $1600^{o}F$(10).

2.2 Properties of LBG

Table 2-1 lists the characteristics of several LBGs produced with several combinations of gasifiers and cleanup systems. The primary combustible species are CO and H_2 comprising 26 to 40 percent with the majority of the remainder composed of H_2, CO_2 and N_2. Approximately half of the LBG is nitrogen introduced into the process as air and this is responsible (in part) for the low gas heating value.

Medium Btu gas with about 400 Btu/ft^3 is produced by replacing the air with oxygen, eliminating the nitrogen.

The ratio CO/H_2 is a function of gasifier design and the steam/air ratio. Typical values range from 0.5 to 2.0.

Table 2-1 also shows that the gasification process converts most of the sulfur to H_2S with the remainder converted to COS. Trace amounts of SO_2, SO_3 and S_2 can also be produced but are not reported in the table. Ammonia, NH_3, is also produced in varying quantities and other nitrogen bearing compounds such as HCN may also be produced but are not reported in the table.

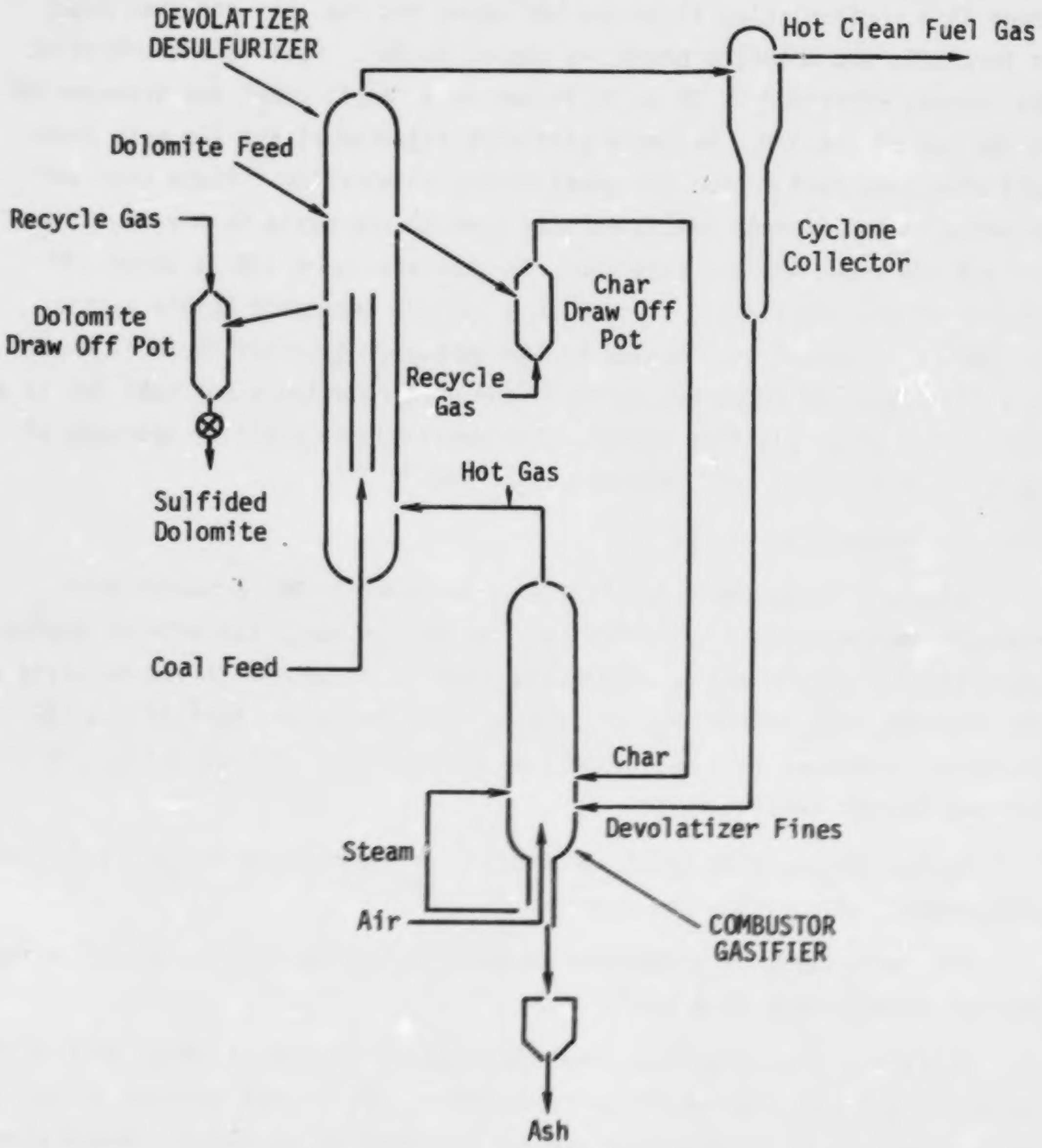
DEVOLATIZER
DESULFURIZER
Hot Clean Fuel Gas
Dolomite Feed
Recycle Gas
Cyclone
Collector
Char
Draw Off
Pot
Dolomite
Draw Off Pot
Recycle
Gas
Hot Gas
Sulfided
Dolomite
Coal Feed
Char
Devolatizer Fines
Steam
Air
COMBUSTOR
GASIFIER
Ash

Figure 2-5. Schematic Diagram of Westinghouse Fluidized Bed Gasifier (from Ref. 10)

Table 2-1. Characteristics of LBG

Name	Lurgi	Bureau of Mines	Bureau of Mines	Bureau of Mines	MERC	Winkler	UGAS	BCR	BCR	BCR	Koppers Totzek
Type of Bed	fixed	fixed	fixed	fixed	fixed	fluidized	fluidized	entrained flow	entrained flow	entrained flow	entrained flow
Cleanup System	None	None	Selexol	Iron oxide	None	None	None	None	Selexol	Conson	None
Temperature			low	high					low	high	
Temperature, ^{o}F	850	1000	265	1070	NR*	2000	1900	1800	1000	1070	1000
Pressure, atm	28.6	34.0	15.8	15.8	10.9	6.8	18.0	34.0	23.8	23.8	34
Higher Heating Value, Btu/ft^3	180	139	NR	NR	104	118	150	125	125	125	139
CO/H_2 Mole Ratio	0.68	1.49	1.49	0.84	1.43	1.62	1.47	1.39	1.42	1.29	1.49
H_2S/COS Mole Ratio	6.0	6.0	NR	NR	NR	NR	NR	4.6	NR	NR	6.0
Mole Fractions											
H_2O	10.1	8.2	0.01	3.9	NR	11.5	12.0	10.5	0.01	9.9	8.24
H_2	19.6	13.8	16.0	18.2	10.7	11.7	11.6	12.0	14.9	13.5	13.8
CO	13.3	20.6	23.9	15.3	15.3	19.0	17.0	16.7	21.2	17.4	20.6
CO_2	13.3	5.9	5.0	11.1	12.7	6.2	8.8	8.8	6.5	9.3	5.9
CH_4	5.5	2.8	3.1	2.8	2.1	0.5	4.1	3.1	4.2	3.6	2.8
H_2S	0.6	0.6	NR	0.01	0.2	0.1	0.6	0.46	NR	NR	0.6
COS	0.1	0.1	0.01	NR	NR	NR	NR	0.1	0.01	0.01	0.1
N_2	37.5	47.6	52.0	47.7	59.3	51.1	45.4	47.7	53.2	45.9	47.6
NH_3	NR	0.15	0.03	0.03	NR	NR	NR	0.38	NR	0.43	0.17
HCN	NR	NR	NR	NR	NR	NR	NR	NR	NR	NR	228 ppm
Reference	3,11	8	12	12	13	11	11	9	12	12	6

---

*NR = Not reported

2.3 LBG Product Gas Cleanup

Low Btu gas leaving the gasifier is termed "dirty" since it contains several materials which can cause environmental problems. A cleanup system is usually installed between the gasifier and combustor to remove these materials. Three types of cleanup systems may be employed:

- particulate removal;
- sulfur removal; and
- nitrogen species removal.

2.3.1 Particulate Removal Systems

Particulate matter in LBG consists of small char and ash particles and its removal is desirable because of the potential for turbine blade erosion downstream of the combustor and atmospheric particulate emission. Since solid and liquid particles are several orders of magnitude more dense than the gaseous constituents, they are usually removed with mechanical equipment. Cyclone separators, electrostatic precipitators and various filters are suitable for this application. Since the gas phase constituents are not affected, particulate removal devices will not be discussed further. Reference 14 summarizes the pertinent aspects of particulate removal systems as applied to LBG.

2.3.2 Sulfur Removal Systems

A variety of sulfur removal systems have been developed or proposed for LBG. All are primarily designed to remove H_2S but may also remove other gases as well. The temperature of the cleanup process is an important consideration and sulfur removal systems may be divided into two categories: low temperature processes requiring gas temperatures less than 250°F, and high temperature processes occurring at or near gasifier outlet temperatures.

Low temperature processes can be subdivided into four groups according to their principle of operation:

- chemical solvent processes,
- physical solvent processes,
- direct conversion processes, and
- dry bed processes.

Table 2-2 compares the characteristics of each type.

Table 2-2. Characteristics of Low Temperature Cleanup Systems (after Colton et al[14])

Basis: 8400 tons/day Illinois No. 6 Coal Fed to BCR Gasifier, or 6700 ppm of Influent H_2S

					Efficiency of S Removal			Absorbent Characteristics				
Process	Absorbent	Type of Absorbent	Temp. °F	Pressure	H_2S Influent	Effluent H_2S ppm	Life	Regeneration	Selectivity Towards	Make up Rate	Form of Sulfur Recovery	Status
CHEMICAL SOLVENT TYPE												
1. MEA	Monoethanol amine	Aqueous solution	80 to 120	Insensitive to variation in pressure	99	~100		Thermal	Forms non-regen, comp. with COS, CS_2	50 to 100%	As H_2S gas	Commercial
2. DEA	Diethanol amine	Aqueous solution	100 to 130	Insensitive to variation in pressure	99	~100		Thermal	Absorbs CO_2, does not absorb COS, CS_2	5%	As H_2S gas	Commercial
3. TEA	Triethanol amine	Aqueous solution	100 to 150	Insensitive to variation in pressure	99	~100		Thermal	H_2S	5%	As H_2S gas	Commercial
4. Alkazid	Potassium dimethyl amino acetate	Aqueous solution	70 to 120	Insensitive to variation in pressure 1-80 atm	99	~100		With Steam	H_2S is high		As H_2S gas	Commercial
5. Benefield	Activated potassium carbonate solution	Aqueous solution	150 to 250		99	H_2S + COS ~100	Unlimited No degradation	With Steam	H_2S - partial also absorbs COS, CS_2	5%	As H_2S gas	Commercial
6. Catacarb	Activated potassium carbonate solution	Aqueous	150 to 250	Insensitive to variation in pressure generally 300 psi	99	H_2S + COS ~100		With Steam			As H_2S gas	Commercial

Table 2-2. (Continued)

					Efficiency of S Removal			Absorbent Characteristics				
Process	Absorbent	Type of Absorbent	Temp. °F	Pressure	H_2S Influent	Effluent H_2S ppm	Life	Regeneration	Selectivity Towards	Make up Rate	Form of Sulfur Recovery	Status
PHYSICAL SOLVENT TYPE												
7. Sulfinol	Sulfolane plus Diisopropanol amine	Organic solvent	80 to 120	High pressure preferred	99	H_2S + COS ~100		Low pressure heating or with steam	H_2S, and also absorbs COS, CS_2 and mercaptans		As H_2S gas	Commercial
8. Selexol	Polyethylene glycol ether	Organic solvent	20 to 80		99	H_2S + COS ~100			H_2S also absorbs COS		As H_2S gas	Commercial
9. Pectisol	Methanol	Organic solvent	0		99	~100			H_2S			Commercial
DIRECT CONVERSION												
10. Stretford	Na_2CO_3 plus anthracuin one sulfonic acid	Alkaline solution			99.9	~10			H_2S	50 to 100	Elemental sulfur	Commercial
11. Townsend	Triethylene glycol	Aqueous solution	150 to 250		99.9	~10			H_2S		Elemental sulfur	Commercial
DRY BED TYPE												
12. Iron sponge	Hydrated Fe_2O_3	Fixed bed	70 to 100		99	H_2S + COS ~100			H_2S and also towards COS, CS_2 and mercaptans		Elemental sulfur	Commercial

Chemical solvent processes employ aqueous solutions to scrub the dirty gas forming complexes with H_2S, CO_2 and other components. The solution is then regenerated at elevated temperatures and recycled. The affinity for CO_2 is undesirable since most LBG contains much more CO_2 than H_2S and CO_2 removal adds unnecessarily to the cleanup system operational cost.

Physical solvent processes utilize absorption rather than chemical reaction to remove certain gas phase species. The absorption is proportional to the partial pressure of the gas to be removed favoring high pressures for good efficiency. These processes selectively remove H_2S over CO_2, and remove other sulfur-bearing species as well.

In direct conversion processes sulfur-bearing species are absorbed in a solvent and reduced directly to elemental sulfur by subsequent reaction. In dry bed processes LBG is forced through a dry bed where sulfur-bearing species are absorbed as solids. These processes are best suited to low concentrations.

In contrast to the low temperature cleanup systems, which can be considered commercial, high temperature desulfurization processes can only be termed "under development". The characteristics of some of the high temperature processes are listed in Table 2-3. None of the processes have been commercialized to date, although the Bureau of Mines Sintered Iron Oxide Process and Consolidated Coal's Half Calcined Dolomite Process will probably be the earliest to claim commercial status. To date, no evidence exists to show that these processes are capable of removing either ammonia or other nitrogen compounds.

Both low and high temperature cleanup processes discussed above can easily remove sulfur compounds from the fuel gas to ensure that total sulfur oxide emissions (from the combustion unit and the sulfur recovery process) are below the allowable SO_2 emissions for large coal-fired power plants (1.2 lb/16^6 Btu).

Table 2-3. Characteristics of High Temperature Cleanup Processes (after Colton, et al[14])

Basis: 8400 tons/day Illinois No. 6 Coal Fed to BCR Gasifier, or 6700 ppm of Influent H_2S

					Efficiency of S Removal		Absorbent Characteristics					Energy Required		
Process	Absorbent	Type of Bed	Temp. °F	Pressure	% H_2S Influent	Effluent H_2S ppm	Life	Regeneration	Selectivity Towards	Make up Rate	Form of Sulfur Recovery	Elec. kW	Other Btu	Status
1. Bureau of Mines	Sintered pellets of Fe_2O_3 (25%) and fly ash	Fixed Bed	1000 to 1500	Insensitive to variation in pressure	~95	~350	>174 cycles wt. loss <5%	With air	H_2S, COS	<5%	As SO_2 gas			Pilot
2. Babcock & Wilcox	Fe_2O_3	Fixed Bed	800 to 1200	Insensitive to variation in pressure	~99	~75					As 12-15% SO_2 gas			Experimental
3. Consolid. Coal	Half calcined dolomite	Fluidized Bed	1500 to 1800	~200 psia H_2S removal is high at low pressure	~95	~350		10-13% with steam and CO_2	H_2S, COS	1% of circulation rate	As H_2S gas to Claus process	96,360		Pilot
4. Air	Calcined dolomite	Fixed Bed	1500 to 2000	Insensitive to variation in pressure			minimum 5-6 cycles	80-90% with steam and CO_2	H_2S, COS		As H_2S gas to Claus process			Abandoned
5. Battelle Northwest	Molten Carbonates (15% $CaCO_3$)	Solution	1100 to 1700	Atmospheric H_2S removal is high at low pressure, 5-6 psig	~95	~350		With steam and CO_2	H_2S, COS, fly ash		As H_2S gas to Claus process			Pilot
6. IST - Meissner	Molten Metal (proprietary)	Splashing contact	900		~98	~150		Electrolytic	H_2S, COS			9,830		Conceptual

2.3.3 Bound Nitrogen Species Removal Systems

The removal of nitrogen-bound species such as NH_3 and HCN from LBG is a difficult problem. Some low temperature sulfur removal systems also remove NH_3, but there are at present no satisfactory high temperature methods.

2.4 Product Gas Combustion Characteristics

As the name implies, the volumetric energy content of LBG is small compared to other common fuel gases such as natural gas. Thus, if LBG is to be substituted for natural gas the pipe supplying the burners must either be larger or operated at higher pressure. Other minor changes include a smaller air supply and smaller wet products of combustion per unit of heat released.

These changes are minor and pose no significant problems in fuel conversion. The major factors determining the suitability of firing LBG in specific furnace designs are flame stability and furnace heat transfer.

2.4.1 Flame Stability

Ball, Smithson, Engdahl and Putnam(15) have discussed the substitution of low Btu gas for natural gas in combustion processes using the critical velocity gradient at flashback as an indication of flame stability*. A flame is stable if the stream velocity and burning velocity are equal at some point along the flame front. If the burning velocity exceeds the stream velocity the flame moves upstream and "flashes back" into the burner. Conversely, if the stream velocity exceeds the burning velocity at every point the flame moves downstream and eventually blows off. Both of these critical gradients (at flashback and blow off) are proportional to the square of the burning velocity (the mass burning rate per unit area of flame surface).

These considerations apply directly to premixed flames but must be modified for the diffusion flames commonly used in utility boilers. Here flame stability results from the recirculation of heat to the base of the flame providing a continual source of reignition. Since maximum flame temperatures are lower with LBG than with natural gas, more recirculation should be necessary to maintain stability. However, burners specifically designed for lean fuel gases have operated satisfactorily for many years and that suggests that flame stability is not a critical problem for LBG.

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*The boundary velocity gradient theory of blow off and flashback was developed by Lewis and von Elbe(16) to correlate stability criterion for premixed flames burning on circular or rectangular ports.

2.4.2 Furnace Heat Transfer

When LBG is substituted for natural gas in a utility boiler it is important that the heat removed from the furnace be the same for both fuels. Since a substantial portion of the heat transfer in a furnace is due to radiation, which is proportional to the fourth power of the radiant gas temperature, the lower flame temperature of LBG could lower furnace heat transfer substantially.

As a first order approximation, Hottel and Sarofim(17) assumed the furnace to be a well-stirred tank and calculated the radiative heat transfer as a function of combustion characteristics. Their model further assumed that:

- the properties of the gases in the furnace are uniform;
- the gas is gray;
- the heat sink has a constant temperature;
- heat losses through the wall are negligible;
- the gases leave the radiant section at a temperature ΔT below the effective radiating temperature of the gases in the furnace T_g; and
- convective heat transfer is negligible compared to radiative loss (although the assumption is later relaxed).

Under these conditions the net heat flux from the gases to the walls $Q_{g\ net}$ is given by:

$$Q_{g\ net} = (GS_1)_R\, \sigma\, (T_g^4 - T_1^4) \qquad (1)$$

$$(GS_1)_R = \frac{A_T}{\frac{1}{\varepsilon_g} + \frac{1}{C_S\,\varepsilon_1} - 1} \qquad (2)$$

where

T_1 is the sink temperature

ε_g is the gas emissivity

ε_1 is the emissivity of the sink surface

C_S is the fraction of the total surface area A_T covered by the sink

If H is the total heat input, $\dot{m}$ is the product mass flow rate, and c_p is the average specific heat,

$$H = \dot{m}\, c_p\, (T_{AF} - T_o) \qquad (3)$$

where T_{AF} is a pseudo adiabatic flame temperature which ignores dissociation. Similarly:

$$H - Q_{g\ net} = \dot{m}\, c_p\, (T_g - \Delta T - T_o) \qquad (4)$$

If the same mean specific heat is assumed then

$$\frac{H - Q_{g\ net}}{H} = \frac{T_g - \Delta T - T_o}{T_{AF} - T_o} \qquad (5)$$

Elimination of T_g between equations (1) and (5) gives

$$\dot{Q}'D' + \tau^4 = (1 + \Delta' - Q')^4 \qquad (6)$$

where

$\dot{Q}' = \frac{Q_{g\ net}}{H}\,\frac{T_{AF} - T_o}{T_{AF}}$ (the dimensionless furnace efficiency)

$D' = \frac{H_F}{\sigma (GS_1)_R\, T_{AF}^3\, (T_{AF} - T_o)}$ (the dimensionless firing density)

$\tau = T_1/T_{AF}$ (the ratio of sink temperature to pseudoadiabatic flame temperature)

$\Delta' = T/T_{AF}$ (the ratio of gas temperature drop to pseudoadiabatic flame temperature)

Equation 6 specified the furnace efficiency as a function of firing density, heat sink temperature and the temperature drop. If the furnace is well-stirred, $\Delta T \rightarrow 0$ and equation (6) simplifies to:

$$\dot{Q}'D' + \tau^4 = (1 - Q')^4 \qquad (7)$$

The results of this analysis may be used to illustrate the difference between firing a furnace with LBG and natural gas. As a simple example consider a utility boiler with a radiant chamber 30' x 60' x 80' high with a total heat input of 300 x 10^6 Btu/hr fired with natural gas with 15 percent excess air at 600°F. T_{AF} is approximately 4140°R and T_1 will be approximately 1160°R if T_g is 3000°F, $\varepsilon_g = 0.38$ and ε_1 the emissivity of the walls is 0.8. Thus:

$$(GS_1)_R = \frac{1800}{2.63 + 1.25 - 1}$$

$$= 6{,}250 \text{ ft}^2$$

$$\tau = \frac{1160}{4140}$$

$$= 0.28$$

$$D' = \frac{300 \times 10^6}{6{,}250\ (0.1712 \times 10^{-8})\ (4140)^3\ 3620}$$

Solving equation (7) iteratively gives:

$$\dot{Q}' = 0.5045$$

and thus the total heat transfer is:

$$\dot{Q}_{net} = 0.5045 \times \frac{4140}{3620} \times 300 \times 10^6 \text{ Btu/hr}$$

$$= 174 \times 10^6 \text{ Btu/hr}$$

If the same furnace were to be fired with LBG produced from a Lurgi gasifier, 600^{0}F preheated air and 10 percent excess air, the pseudoadiabatic flame temperature would be 3,560^{0}R. Therefore,

$$D' = 0.204$$

$$\dot{Q}' = 0.4427$$

$$\dot{Q}_{net} = 153 \times 10^6 \text{ Btu/hr}$$

These approximate calculations give some indication of the radiatability of LBG compared to natural gas.

As expected, the furnace heat transfer with LBG is lower. However, the difference is not large, particularly considering the approximations involved. If the furnace was to be designed specifically for LBG, the radiative section should be slightly enlarged over natural gas designs.

2.5 Low Btu Gas Combustion – Pollutant Emissions

Carbon monoxide and nitrogen oxides are the atmospheric pollutants most likely to be formed during the combustion of coal-derived LBG. Nitrogen oxide formation is a natural consequence of efficient combustion, whereas the emission of significant quantities of carbon monoxide is an indication of poor combustion conditions. Carbon monoxide emissions can be prevented by providing complete fuel/air mixing and avoiding rapid quenching of the combustion products.

Nitrogen oxides can be produced from two sources:

- the oxidation of molecular nitrogen (thermal NO); and
- the oxidation of nitrogen-bearing compounds (such as ammonia in LBG)

The reactions forming NO from molecular nitrogen are of two types: the reactions originally proposed by Zeldovich, and those in which the nitrogen molecules are attacked by hydrocarbon fuel fragments producing nitrogen intermediaries which subsequently form NO. The production of NO from nitrogen-bearing compounds is controlled mainly by the availability of oxygen, although temperature also has some effects. The adiabatic flame temperatures of low

Btu fuel gases are relatively low, and thus their potential to form thermal NO is also low. However, fuel NO formation is almost independent of flame temperature and relatively high conversions of NH_3 to NO are expected, particularly with vigorous fuel/air mixing.

Rawdon et al[(18)] have recently burned both medium and low Btu fuel gas in an experimental tunnel furnace using a typical boiler burner and measured NO emissions. Thermal NO levels between 80 and 150 ppm were measured and thermal NO levels between 50 and 60 ppm were reported for a turbo furnace burning 90 Btu/ft^3 blast furnace gas. Conversions of NH_3 to NO from 60 to 20 percent were reported for NH_3 concentrations of 0.04 and 0.2 percent. Thus the presence of ammonia in coal-derived LBG may cause significant NO emissions.

3.0 ADVANCED POWER GENERATING SYSTEMS ANALYSIS

Power plants fired with coal-derived LBG will only be competitive with conventional direct-fired power plants if the capital costs and energy losses in the gasification process are countered by plant improvements such that the overall efficiency and cost of electricity are comparable. Furthermore, since these improvements may drastically alter the combustion parameters, it is important to identify those advanced power generating systems with the best performance and those most likely to be constructed based on economic considerations.

This section discusses a comparative analysis of several advanced power generating systems based on separate sets of assumptions:

- Separate gasifier and power plant — fuel transfer from gasifier to power plant is the only coupling. All components are representative of existing technology with no advances in the state-of-the-art.
- Integrated gasifier/power plant combined cycle system with heat, and mass and fuel transferred between the components, and each component optimized for optimum overall system performance.

An analysis based on the first set of assumptions was conducted by Combustion Engineering under subcontract to Ultrasystems. This approach is reasonable as a first approximation and applies directly to situations where the gasification complex and power plant must be separated by some distance or cannot be directly integrated into the power plant for other reasons. The next section discusses the results of this study.

Integrating the gasifier into the power plant and optimizing each component can improve overall systems performance substantially, but would require some development work extending the state-of-the-art in gasifier and power plant design and a careful analysis of the entire power plant to identify optimums. Consequently, the results of the second analysis apply to more advanced future power plants to be constructed some time in the mid to late 1980s. The results are presented in Section 3.2.

3.1 Separate Gasifier/Power Plant Comparative Analysis

This section presents the results of a comparative analysis of LBG-fired power plants conducted by Combustion Engineering under subcontract to Ultrasystems. Two basic restrictions were imposed upon the power generating systems:

- An integrated gasifier-power plant system was not to be considered. The fuel was to be purchased "over the fence".
- All components in the system must represent existing technology and require no advances in the state-of-the-art.

Systems meeting these requirements were then assumed to be fired with two alternative fuels representative of existing coal gasification technology:

- A fuel gas typical of that produced by a large air-blown Lurgi gasifier; and
- A medium heating value fuel typical of that produced by an oxygen-blown Koppers Totzek (K-T) system.

The compositions assumed for these fuels are given in Table 3-1.

Table 3-1. Fuel Gas Compositions

Component	Low Btu Lurgi	Medium Btu (K-T)
CO	14.1 vol percent	53 vol percent
H_2	20.9	36.4
CH_4	5.8	– –
CO_2	12.5	9.25
H_2O	6.6	0.3
N_2	40.1	1.05
LHV (Btu/scf)	172	272
60°F and 1 atmosphere		

Both fuels were assumed to be delivered to the power plant at up to 1500°F and 10 atmospheres.

The study began with a preliminary screening of 35 conceptual power plants and six were chosen for further detailed analysis. These plants were then analyzed thermodynamically to determine heat and material balances and to calculate overall plant performance at design point. The capital and operating costs were also estimated to identify the most cost-effective designs. Finally, the combustion conditions, heat transfer surface areas and special materials for each type of combustion were determined.

3.1.1 Preliminary Screening

Thirty-five conceptual power plant systems were considered in the preliminary screening. These concepts can be conveniently classified into the following groups:

- Conventional steam power plant with or without fuel gas precooling or high temperature burners.
- Combined cycle systems with waste heat or supplementary-fired steam boilers
- Supercharged boiler combined cycle systems
- Combustors fired by oxygen for those systems with medium Btu gas (since oxygen is required for the gasificiation process)

A complete description of each system is given in Appendix A and the major findings are summarized in Table 3-2. The twelve most promising systems were provisionally selected for more detailed consideration and are listed below:

A1	Conventional plant baseline case
B1	High temperature fuel gas and precooler
G3	Supplementary-fired combined cycle
G5	Supplementary-fired combined cycle with fuel gas cooler
G1	Supplementary-fired combined cycle with fuel gas cooler
G2	Supplementary-fired combined cycle with fuel gas cooler
H1	Supercharged boiler combined cycle
E5	Exhaust-fired combined cycle
C1	Conventional power plant with high temperature burners
H2	Supercharged boiler with process steam fuel gas precooler
I1	Oxygen-fired supercharged boiler
I4	Oxygen-fired supercharged boiler fuel gas precooler

Table 3-2. Summary of Preliminary System Concept Analysis

Class	Description	No.	Fuel Gas Press.	Fuel Gas Temp.	Remarks
A	Conventional Utility Steam Power Plan	1	Low	Low	Baseline system, all components of current design, low NO_x potential, retrofit possible, but high capital cost.
		2	High	Low	High pressure fuel more suited to combined cycle, otherwise fuel throttling loss.
B	Conventional Power Plant with Gas Precooler	1	Low	High	Components of current design, produces process steam in quantities dependent upon load.
		2	Low	High	Uses hot fuel as air heater, explosive potential of gas precooler, retrofit unlikely.
		3	High	High	Fuel throttling loss.
C	Conventional Power Plan with High Temperature Burners and Partial Precooling	1	Low	High	Burner development could be required, possible NO_x problems
		2	Low	High	Partial precooler producing process steam burner development not warranted.
		3	Low	High	Partial gas precool to heat air.
D	Industrial Boiler Systems	1	Low	Low	All have high plant heat rates, complex system design, marginal delivery time and cost advantage may require new steam turbine design.
		2	Low	High	
		3	High	High	
		4	High	Low	

Table 3-2 (Continued)

Class	Description	No.	Fuel Gas		Remarks
			Press.	Temp.	
E	Waste Heat Boiler Combined Cycle Systems	1	Low	Low	Higher plant heat rates than corresponding G systems, good load demand flexibility
		2	Low	High	
		3	High	Low	
		4	High	High	High NO_x potential
		5	High	High	Low NO_x because of process steam heater
F	Exhaust-Fired Boiler Combined Cycle Plant	1	Low	Low	No advantage to offset higher plant heat rates than G systems
		2	Low	High	
		3	High	Low	
		4	High	High	
		5	High	High	
G	Supplementary-Fired Boiler Combined Cycle Plant	1	Low	Low	Low plant heat rate, components are of current design, low NO_x potential
		2	Low	High	
		3	High	Low	
		4	High	High	High NO_x potential because of hot fuel gas
		5	High	High	
H	Supercharged Boiler	1	High	Low	Compact design, low heat rate plant, lower capital cost, existing technology but not widely used in the U.S., NO_x unknown.
		2	High	High	
		3	Low	Low	System design not warranted for low pressure fuel.
		4	Low	High	
I	Supercharged Boiler Combined Cycle Oxygen	1	High	Low	As for systems H, but cost of oxygen may affect any advantage.
		4	High	High	
		3	Low	Low	
		2	Low	Low	

Robson, et al[7,8,9] has made extensive studies on the utilization of coal-derived fuel gas in waste heat and supplementary-fired boiler combined cycle systems. Consequently, to prevent repetition it was decided to eliminate systems G and E from further consideration, and to concentrate upon four variations from conventional utility power plant technology:

- The use of a gas/water heat exchanger to cool the fuel gas and produce process steam.
- The use of high temperature burners in a conventional boiler.
- The use of oxygen (instead of air) with a medium heating value gas.
- A supercharged boiler combined cycle steam plan.

The six systems listed in Table 3-3 were selected for detailed analysis. The first two are conventional power plants fired with the two fuel gases and the other four represent the four variations listed above.

3.1.2 System Design

Each of the six systems selected for detailed analysis was developed and optimized for a 500 MW plant with an acceptably low overall plant heat rate in keeping with usual engineering practice and the limitations of state-of-the-art components.

This required an increase in plant complexity and capital cost because of certain special characteristics of LBG such as the low air/fuel ratios which necessitated stack gas coolers. A simplified schematic diagram and heat and material flows for each system are shown in Figure 3-1 through 3-6, and Table 3-4 summarizes the major components.

All plants except system H1-L (supercharged boiler combined cycle) utilize a single, conventional balanced draft, controlled circulation boiler producing a maximum of 3,310,000 lbs/hr main steam flow with superheat and reheat steam conditions of 1011°F/2685 psig and 1101°F/501 psig respectively. Superheat steam temperature control is via burner tilt or gas recirculation. The furnace is single cell with tangential or alternate opposed wall burner designs. Extremely high gas recirculation (205 percent) was included for

Table 3-3. Summary of Systems Studied During Critical Analysis

Description	System	Fuel Properties (as Purchased)			Remarks
		Type	Pressure psig	Temp. °F	
Conventional Plan	A1-L	Low Btu (Lurgi)	10	250	Baseline
Conventional Plan	A1-K	Medium Btu (Koppers)	10	250	Baseline
Conventional Plan with Precooler	B1-L	Low Btu (Lurgi)	10	1500	Fuel enters the plant at 1500°F, is cooled to 750°F in a waste heat boiler and fired through conventional burners.
Conventional Plant with High Temperature Burners	C1-L	Low Btu (Lurgi)	10	1500	Fuel enters the plant at 1500°F and is fired through high temperature burners.
Supercharged Boiler Combined Cycle	H1-L	Low Btu (Lurgi)	132	654	Furnace pressure 10 atmsopheres. Turbine inlet temperature 2000°F producing 33 percent of the power output.
Conventional Boiler with O_2	I5-K	Medium Btu (Koppers)	10	250	Air for combustion replaced by oxygen.

SYSTEM A1-L

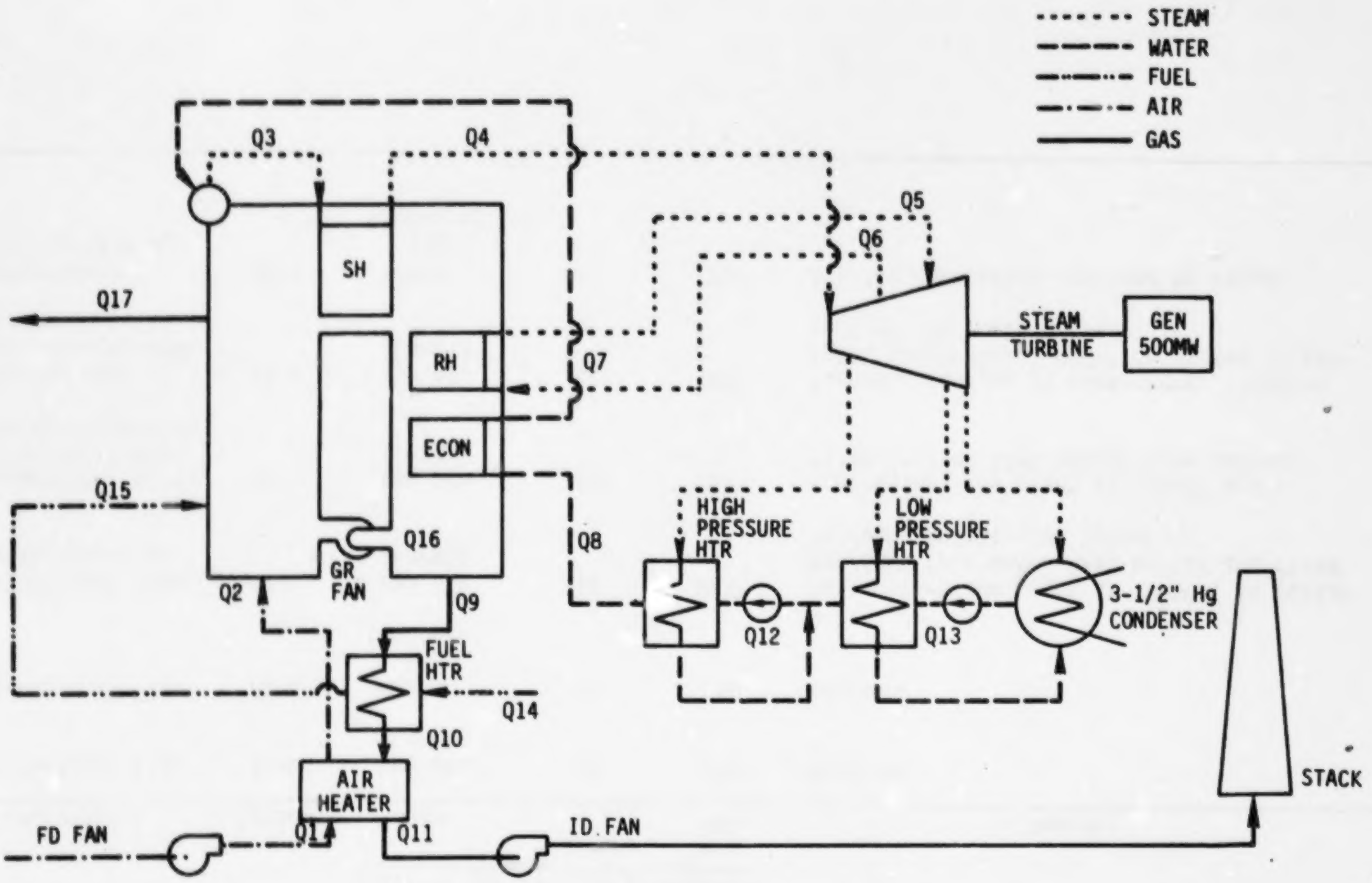
STEAM
WATER
FUEL
AIR
GAS
Q3
Q4
Q5
Q6
SH
Q17
RH
Q7
STEAM
TURBINE
GEN
500MW
ECON
Q15
HIGH
PRESSURE
HTR
LOW
PRESSURE
HTR
Q16
Q8
GR
FAN
Q2
Q9
Q12
Q13
3-1/2" Hg
CONDENSER
FUEL
HTR
Q14
Q10
AIR
HEATER
STACK
FD FAN
Q1
Q11
ID FAN

Figure 3-1. Conventional Steam Plant, System A1, Lurgi LBG, Low Temperature

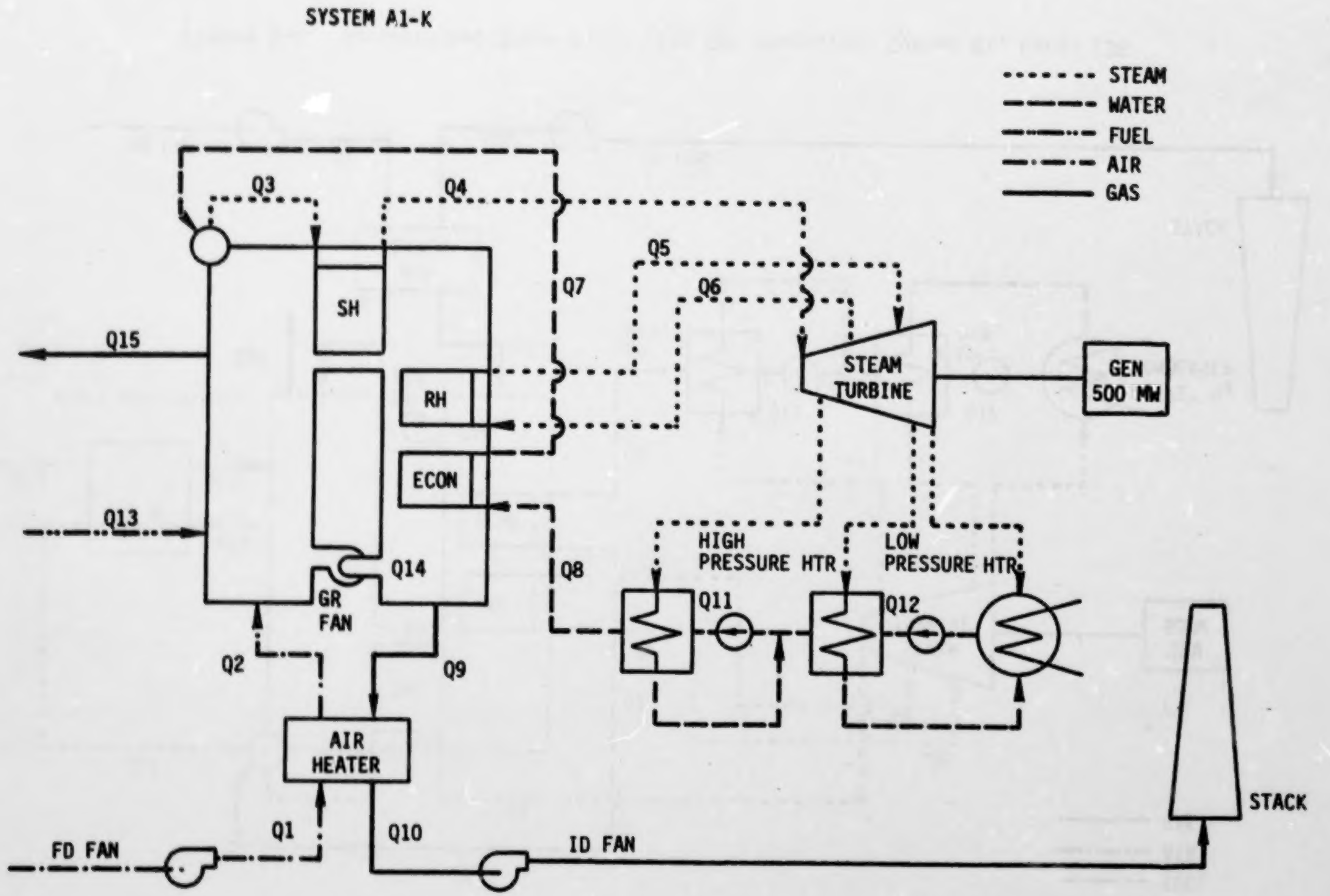
SYSTEM A1-K
STEAM
WATER
FUEL
AIR
GAS
Q3
Q4
Q5
Q6
Q7
SH
RH
ECON
Q15
Q13
Q14
GR
FAN
Q8
STEAM
TURBINE
GEN
500 MW
HIGH
PRESSURE HTR
LOW
PRESSURE HTR
Q11
Q12
Q2
Q9
AIR
HEATER
Q1
Q10
FD FAN
ID FAN
STACK

Figure 3-2. Conventional Steam Plant, System A1, Koppers Totzek MBG, Low Temperature

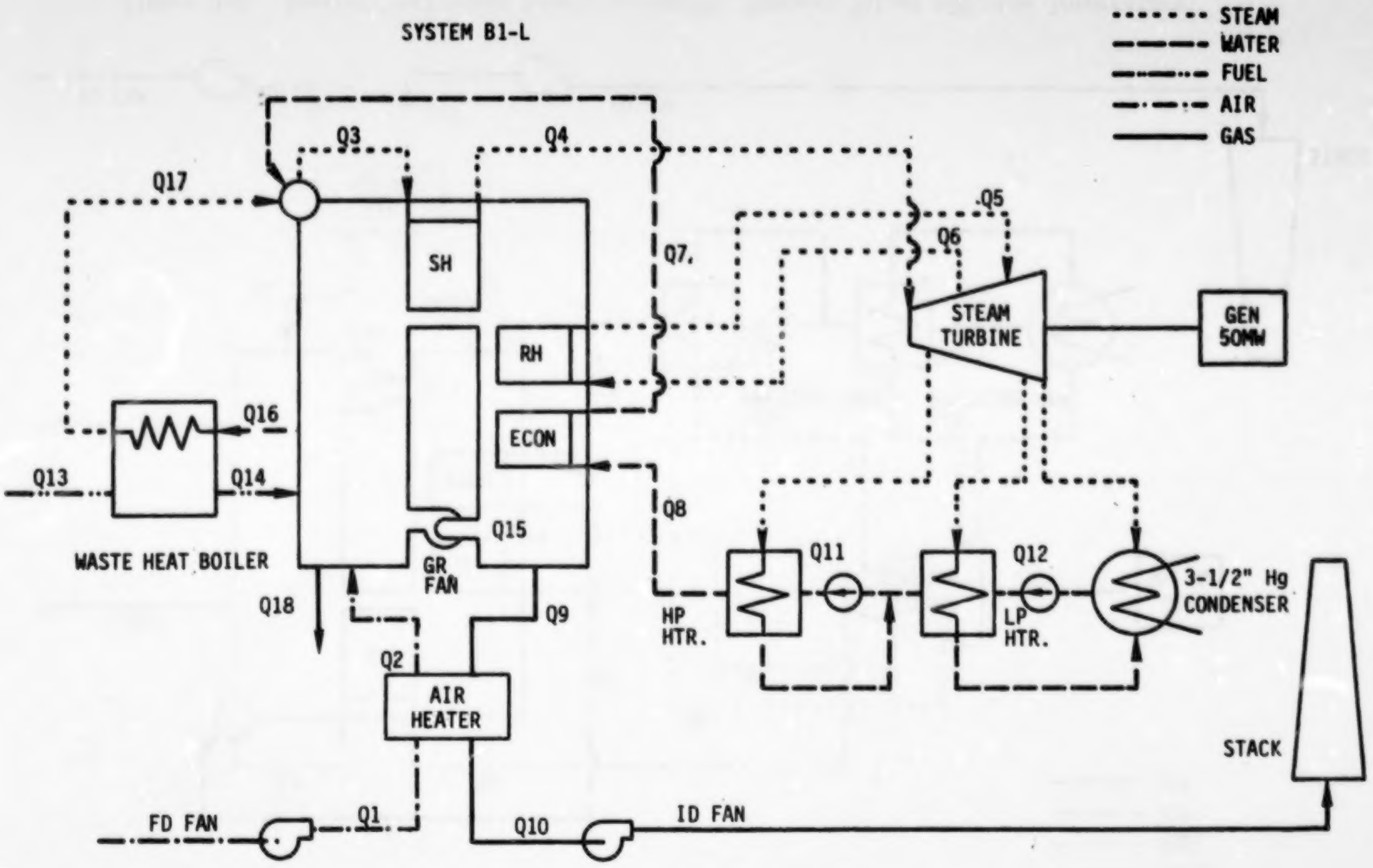
SYSTEM B1-L
STEAM
WATER
FUEL
AIR
GAS
Q17
Q3
Q4
SH
Q7.
.Q5
Q6
STEAM TURBINE
GEN 50MW
RH
ECON
Q16
Q13
Q14
Q15
Q8
WASTE HEAT BOILER
GR FAN
Q18
Q9
Q2
AIR HEATER
Q11
Q12
HP HTR.
LP HTR.
3-1/2" Hg CONDENSER
STACK
FD FAN
Q1
Q10
ID FAN

Figure 3-3. Conventional Steam Plant with Gas Precooler, System B1, Lurgi LBG

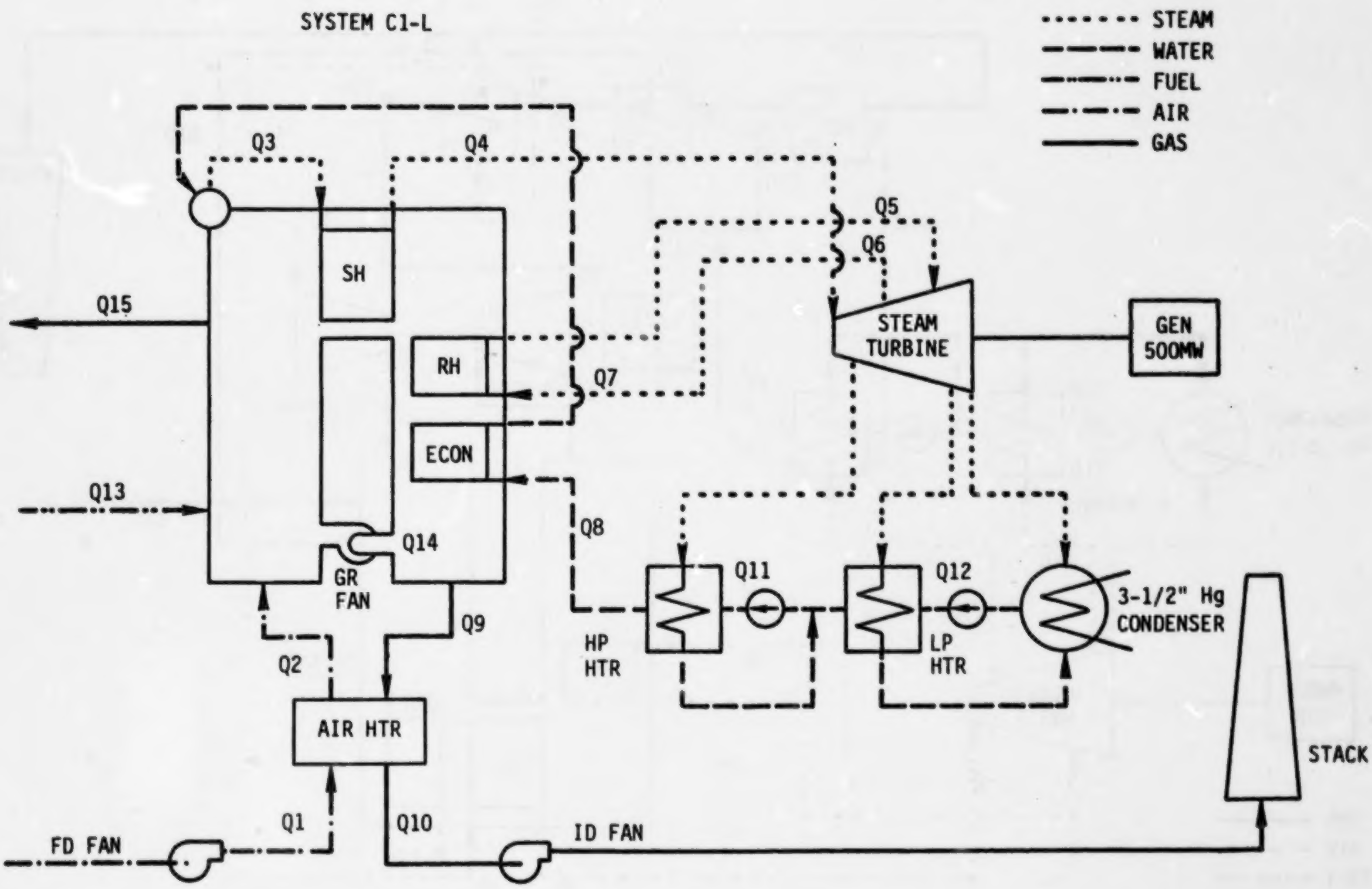
SYSTEM C1-L
STEAM
WATER
FUEL
AIR
GAS
Q3
Q4
Q5
Q6
Q7
Q8
Q9
Q10
Q11
Q12
Q13
Q14
Q15
Q2
Q1
SH
RH
ECON
GR
FAN
AIR HTR
FD FAN
ID FAN
STEAM
TURBINE
GEN
500MW
HP
HTR
LP
HTR
3-1/2" Hg
CONDENSER
STACK

Figure 3-4. Conventional Steam Plant with High Temperature Burners, System C1, Lurgi MBG, High Temperature

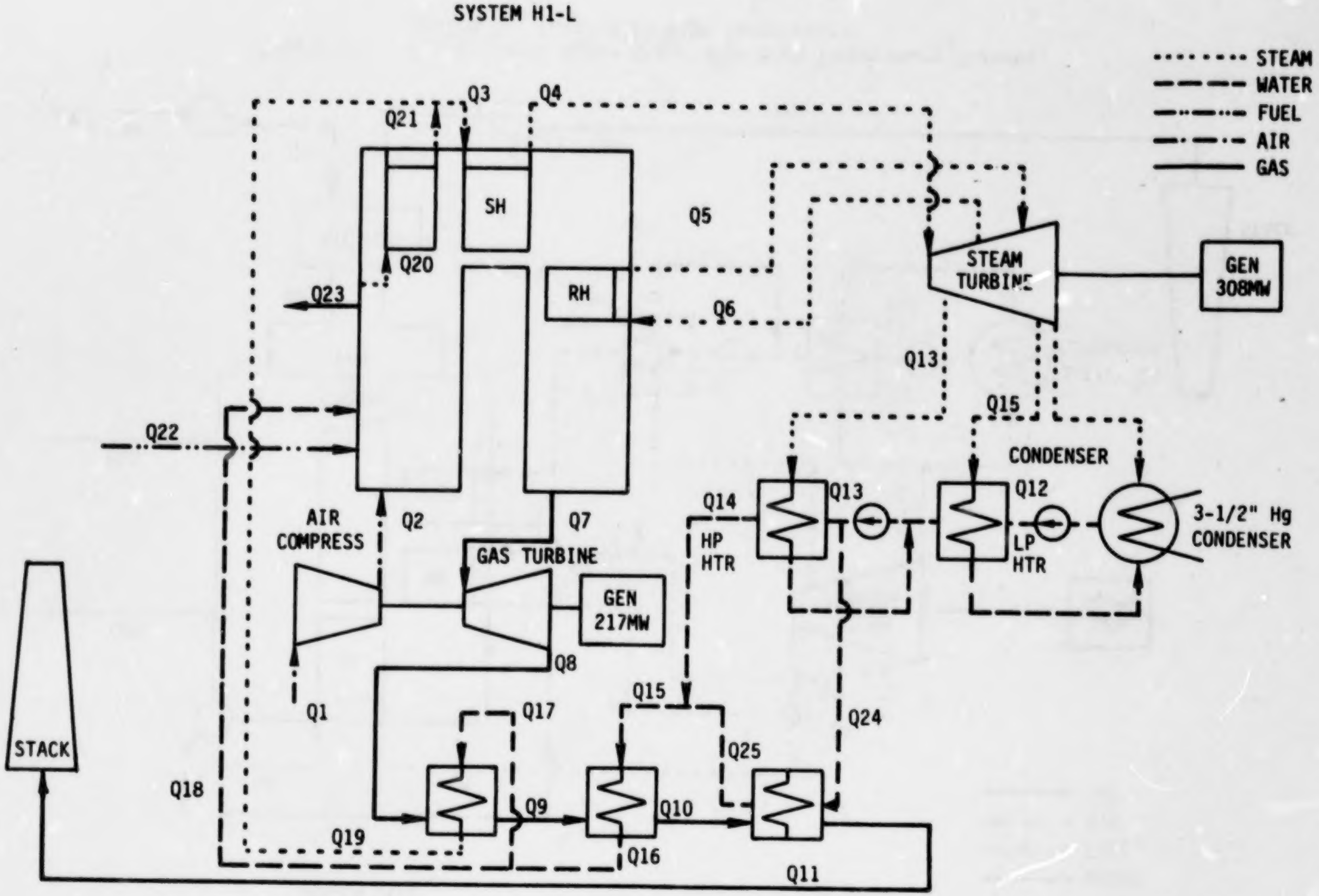
SYSTEM H1-L
STEAM
WATER
FUEL
AIR
GAS
Q3
Q4
Q21
SH
Q5
Q20
Q23
RH
Q6
STEAM TURBINE
GEN 308MW
Q13
Q15
CONDENSER
Q22
Q14
Q13
Q12
3-1/2" Hg CONDENSER
AIR COMPRESS
Q2
Q7
GAS TURBINE
HP HTR
LP HTR
GEN 217MW
Q8
Q1
Q15
Q17
Q24
Q25
STACK
Q18
Q9
Q10
Q19
Q16
Q11

Figure 3-5. Supercharged Boiler Combined Cycle, System H1, Lurgi LBG

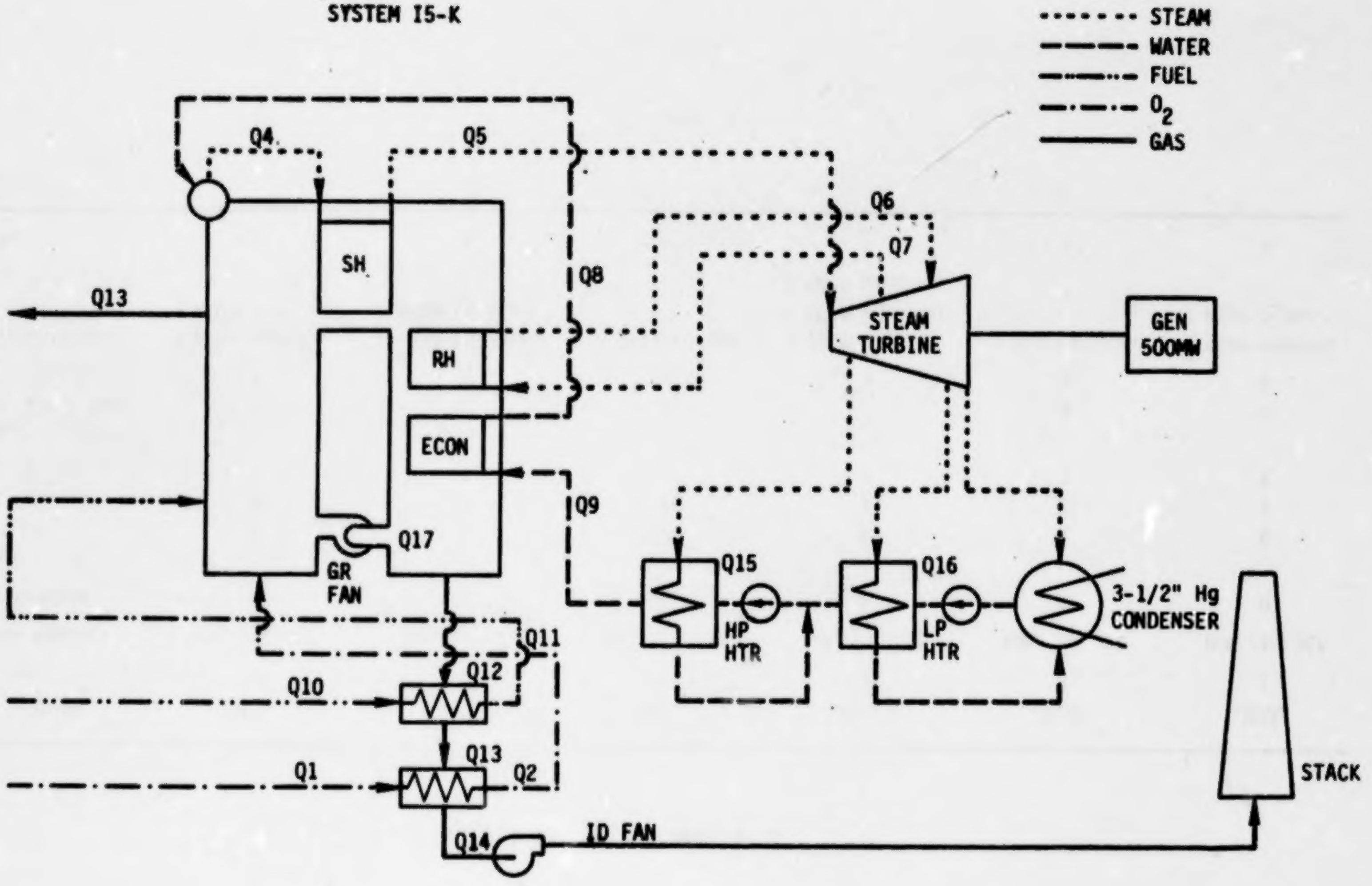
SYSTEM I5-K
STEAM
WATER
FUEL
O_2
GAS
Q4
Q5
Q6
Q7
Q8
Q9
SH
RH
ECON
Q13
Q17
GR FAN
STEAM TURBINE
GEN 500MW
Q15
HP HTR
Q16
LP HTR
3-1/2" Hg CONDENSER
Q11
Q12
Q10
Q13
Q1
Q2
Q14
ID FAN
STACK

Figure 3-6. O_2 Blown Steam Plant, System I5, Kopper Totzek MBG

Table 3-4. Major Components

System	A1-L	B1-L	C1-L	H1-L	A1-K	I5-K
Boilers	1	1	1	3	1	1
Steam Turbines	1HP, 1IP, 2LP	1HP, 1IP, 2LP	1HP, 1IP, 2LP	1HP, 1IP, 2LP	1HP, 1IP, 2LP	1HP, 1IP, 2LP
Gas Turbines	0	0	0	3	0	0
Fans:						
FD	2	2	2	0	2	0
ID	2	2	2	0	2	2
GR	1	1	1	0	1	2
Pumps:						
Boiler Feed	2	2	2	2	2	2
Circ.	3	3	3	0	3	3
Special Heaters	2 RECUP Fuel/Gas 2 REGEN Air/Gas	2 RECUP Fuel/Steam 2 REGEN Air/Gas	2 REGEN Air/Gas	3 RECUP Steam/Gas 3 RECUP Water/Gas 2 RECUP Water/Gas	2 REGEN Air/GAS	2 RECUP FUel/Gas 2 RECUP O_2/Gas
Stack	1	1	1	2	1	1

the O_2 Blown Steam Plant (System I5-K), in order to maintain peak gas (and hence, metal) temperatures within acceptable limits. The major differences between these boilers and conventional LBG boilers are the fuel piping, the burners, stack gas coolers and the introduction of flue gas recirculation through the windbox instead of through the hopper bottom.

The Supercharged Boiler Combined Cycle Plant (System H1-L) includes three 10 atmosphere once-through boilers. A side elevation through one possible design is presented in Figure 3-7. The LBG fuel would be fired through a single fixed vane (SV) burner in the bottom of each furnace. Each of the boilers has a maximum continuous rating of 612,000 lbs/hr main steam flow with superheat and reheat steam conditions the same as the other plants. Superheat and reheat steam temperature control is achieved via desuperheat spray. Flue gas leaves the boilers at 2000°F and is delivered to three gas turbines; heat losses from the system are minimized by routing the air from the compressors to the boilers in an annulus surrounding the flue gas pipe. Upon leaving the gas turbines the flue gas passes through a waste heat recovery chain consisting of an evaporator-superheater, economizer and a feedwater heater. The flue gas at 300°F then passes to the stack. The three gas turbine generator sets deliver a total net output of 191 MW; a single steam turbine generator delivers 308 MW net.

3.1.3 Plant Optimization and Performance

The optimization of each of the six systems was relatively straightforward with the possible exception of the combined cycle system number H1-L. The desire for high plant efficiency, low stack temperature and the limitations of existing materials and components dictated the plant arrangements.

The optimization of the combined cycle system number H1-L was somewhat more complex. The relationships between gas turbine inlet temperature, pressure ratio (or equivalently furnace pressure) and plant net heat rate holding stack temperature and steam turbine output constant are shown in Figure 3-8*. The plant heat rate is seen to improve with increasing turbine

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*Heat rate is the number of Btus required to provide 1.0 kWh of electricity and is inversely proportional to overall efficiency.

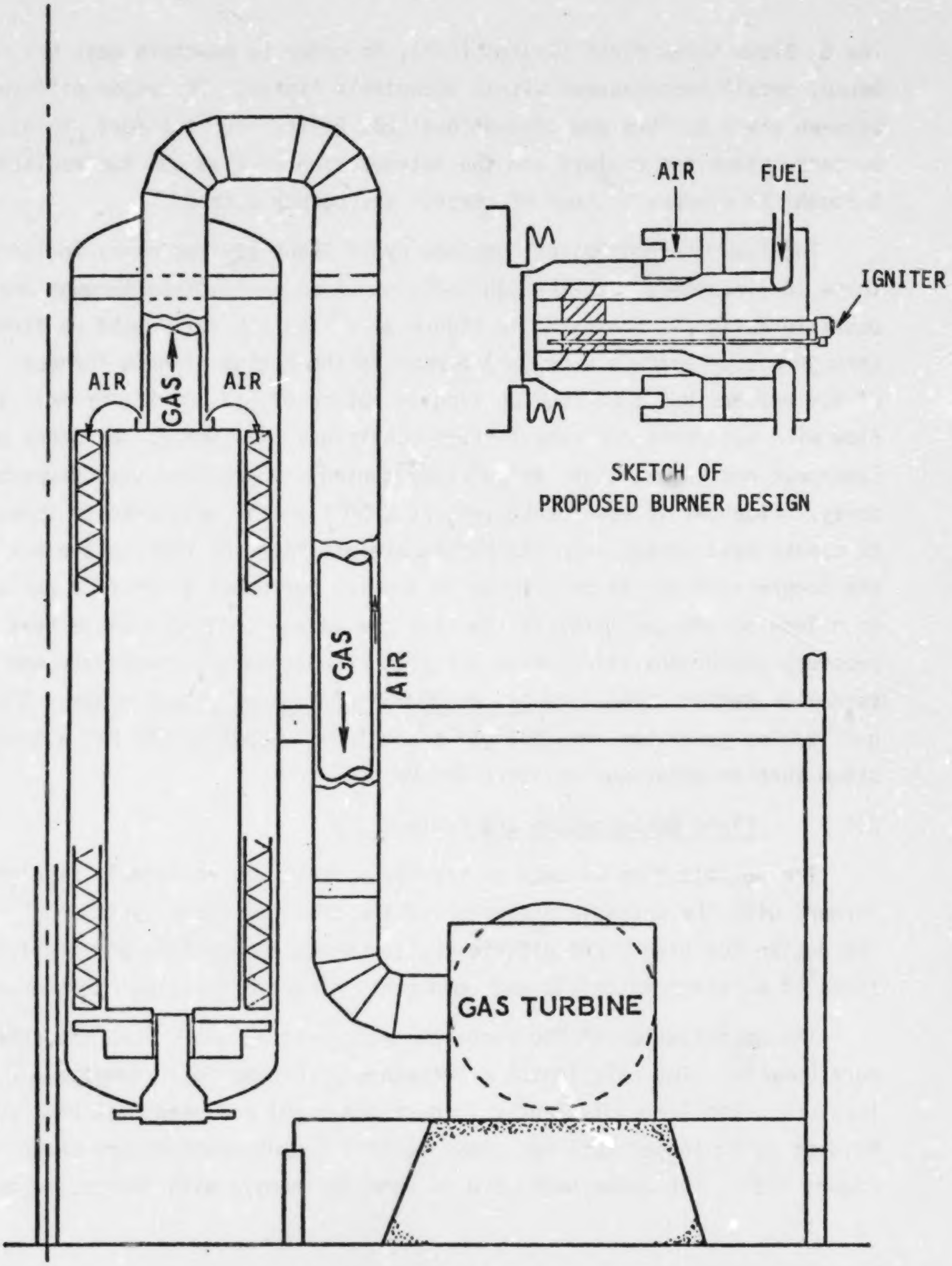
AIR
FUEL
IGNITER
SKETCH OF
PROPOSED BURNER DESIGN
AIR
GAS
AIR
GAS
AIR
GAS TURBINE

Figure 3-7. Side Elevation Showing Detail of Supercharged Boiler and Burner

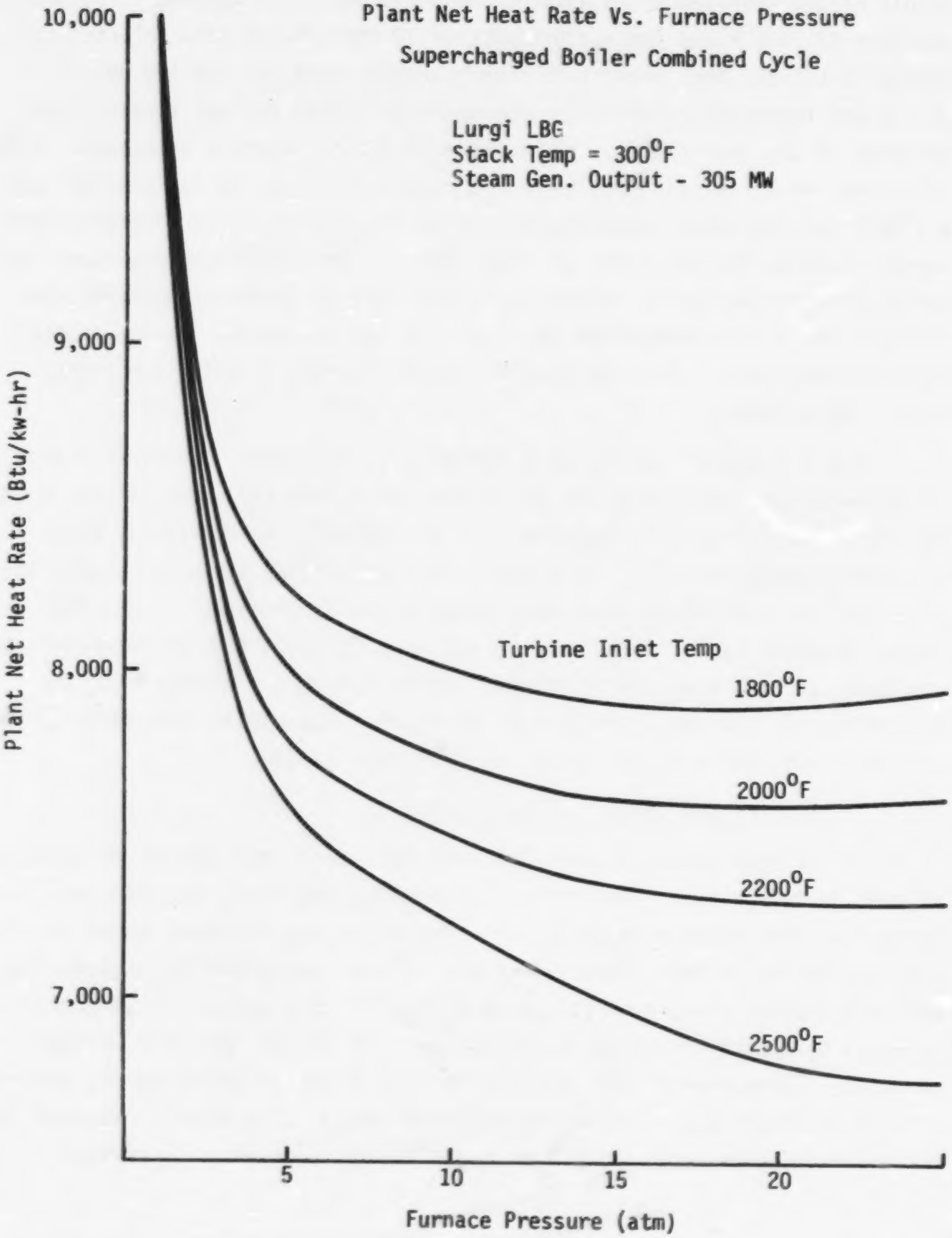

Figure 3-8. Plant Heat Rate as a Function of Furnace Pressure and Turbine Inlet Temperature

inlet temperature and furnace pressure (within the range indicated), a direct result of the improvement in gas turbine performance. A turbine inlet temperature of 2000°F and furnace pressure of 10 atmospheres were selected for System H1-L since they present no insurmountable problems for the boiler design and represent conservative estimates of industrial gas turbine capabilities in the near future. For example, G.E. is currently offering a 70 MW oil-fired industrial gas turbine with a compressor pressure ratio of 9.7 and a 1950°F turbine inlet temperature; United Aircraft has built several slightly larger machines which operate at these levels. The 2000°F turbine inlet temperature selection may be conservative since the characteristic temperature "spikes" found for conventional machines are not present for this combustor/boiler arrangement. Thus the turbines should be able to withstand higher inlet temperatures.

Table 3-5 summarizes the performance of each system. The overall plant efficiencies and heat rates for all plants are nearly the same with the exception of the combined cycle plant number H1-L which is substantially better. Since this analysis assumed no integration of gasifiers and power plant, the efficiencies, heat rates, etc., are based on the heat content of the fuel gas rather than the parent coal. The overall gasifier and plant performance from coal pile to busbar must also consider gasifier losses. Systems B1-L and C1-L which utilize the sensible heat of the fuel gas should have 10 to 15 percent improved gasifier efficiency over the other systems.

3.1.4 Capital and Operating Cost Estimates

Capital cost estimates were prepared for each of the systems by assuming an average U.S. site. Plant capital costs including field erection, are summarized in 1974 dollars in Table 3-6 using the standard Federal Power Commission accounting system. Twenty-four percent has been added for engineering and construction management (13 percent) and for contingency (11 percent). Interest during construction is calculated at an annual rate of 8 percent using an S-curve expenditure schedule for four years of construction, giving a total of 17 percent. The total estimated cost is also shown in dollars per net kilowatt. These cost estimates are within plus or minus 10 percent.

Table 3-5. Plant Performance

System	A1-L	B1-L	C1-L	H1-L	A1-K	I5-K
Net Power Plant Eff. %	36.2	36.3	36.3	43.7	37.8	38.3
Net Power Plant Heat Rate Btu, 1 kW/hr	9440	9420	9420	7814	9040	8920
HHV Heat Energy Input 10^6 Btu/hr	4720	4710	4710	3899	4520	4460
New Power Plant Output MW	500	500	500	499	500	500
Steam Turbine Output MW	500	500	500	308	500	500
Steam Turbine						
Throttle Conditions psia/^{o}F/^{o}F	2535/1000/1000	2535/1000/1000	2535/1000/1000	2535/1000/1000	2535/1000/1000	2535/1000/1000
Steam Turbine Back Press., Inch Hg.	3.5	3.5	3.5	3.5	3.5	3.5
Gas Turbine Power Output, MW	---	---	---	191	---	---
Gas Turbine Inlet Temp., ^{o}F	---	---	---	2000	---	---
Gas Turbine Back Press., psia	---	---	---	15.2	---	---
Power Plant Aux. Power, MW	17.4	17.4	17.4	5.2	15.4	16.4
Stack Temp., ^{o}F	250	300	300	300	250	350
Steam Turbine Output, %	100	100	100	61.7	100	100

Table 3-6. Plant Capital Costs

Plant Number	A1-L	B1-L	C1-L	H1-L	A1-K	I5-K
Land and Land Rights	572	571	571	557	570	571
Structure & Improvement	16,900	16,900	16,900	15,900	16,900	16,900
Boiler Plant Equip.	38,900	38,970	36,440	27,400	36,020	36,020
Turbine Gen. Equip.	26,500	26,400	26,400	32,300	26,300	26,400
Accessory Elec. Equip.	1,100	1,100	1,100	1,150	1,100	1,100
Misc. Power Plant Equip.	1,450	1,450	1,450	1,830	1,450	1,450
Station Equip.	1,300	1,300	1,300	1,360	1,300	1,300
Subtotal	86,812	86,691	84,161	80,497	83,640	83,741
Engineering, Design Const. Management, Temp. Const. Facilities & Contingency	20,835	20,806	20,199	19,319	20,074	20,098
Subtotal (1974)	107,647	107,497	104,359	99,817	103,713	103,839
Escalation (1974)	-0-	-0-	-0-	-0-	-0-	-0-
Interest During Const.	18,300	18,274	17,741	16,969	17,631	17,653
Total Estimated Cost	125,947	125,771	122,101	116,786	121,344	121,491
Estimated Cost /Net KW	252	252	244	234	243	243

Capital costs for equipment in Combustion Engineering's scope of supply were estimated by C.E. This includes boilers, fans, economizers, air heaters, steam and feedwater piping, stacks, etc. These items are all included in boiler plant equipment. Land is included at typical costs for average U.S. sites. The balance of the equipment for the plants was cost estimated by scaling previous consulting engineering firm estimates for similar plants. The combined cycle plant number H1-L has steel stacks supported on the steel work of the waste heat recovery sections and the remainder of the plants each have a single concrete stack. Stack dimensions are summarized below:

System	Stack Height (ft)	Stack Diameter (ft)
A1-L	260	23.8
B1-L	210	22.1
C1-L	210	22.1
A1-K	260	20.8
I5-K	180	15.0

Structures and improvements include site improvements, buildings, and foundations. Boiler plant equipment costs are significantly less for the combined cycle System H1-L due to reduced steam.

Turbine generator equipment includes steam turbines and generators, condensers and auxiliaries, circulating water system, cooling towers, make up water system, steam turbine auxiliaries, gas turbines and generators and gas turbine auxiliaries. The gas turbines in the combined cycle plant, H1-L result in higher costs in this area, but these are more than offset by the lower boiler plant equipment costs.

Accessory Electrical Equipment includes auxiliary power transformers, switchgear and buses, electrical control board, relay boards, motor control boards, and miscellaneous substations. These cost totals are essentially the same for all plants.

Miscellaneous power plant equipment includes laboratory and sampling equipment, tools, lockers, emergency equipment, portable cranes and hoists, and communication equipment. This equipment costs more for the combined cycle plant H1-L due to the addition of gas turbines.

Station equipment includes the main power transformers, buses, and insulators. The cost for the combined cycle plant H1-L is slightly larger than the other plants due to the increased number of generators.

Performance and operating costs for 1974 operation are summarized in Table 3-7 and the details of the calculations are listed in Table 3-8. The gross electrical output is approximately 520 MW for each plant after correcting for typical auxiliary power requirements including condenser cooling pumps, boiler circulating pumps, FD, ID and GR fans, and transformer losses (0.5 percent of the net output). The boiler feed pumps are steam turbine driven and are included in the steam cycle. The net plant heat rate is the gross (higher heating value plus sensible) fuel heat input divided by the net output. Annual net generations are the net full load output times 5000 and 7500 hours per year. These are equivalent to load factors of 57 and 86 percent. Capital costs are from Table 3-8. A fixed charge rate of 20 percent of capital cost per year is assumed as typical for an average U.S. site.

Annual fuel costs for 1974 are based on $\$1.25/10^6$ Btu as the delivered price for 10 psig Lurgi LBG and $\$1.40/10^6$ Btu for 147 psig Lurgi LBG. The delivered price for Koppers Totzek MBG is $\$1.50/10^6$ Btu. Plant I5 has an additional cost of $\$0.55/10^6$ Btu for oxygen for the boiler, resulting in a total of $\$2.05/10^6$ Btu. These costs are based upon estimates of coal and gasification costs. For example, Koppers Totzek estimates the cost of 300 Btu/ft^3 fuel gas at $\$1.00/10^6$ Btu based on coal available at $\$0.80/10^6$ Btu. However, recent coal costs are as high as $\$1.60/10^6$ Btu. The best price for a long-term, large volume contract for 3 percent sulfur bituminous coal is currently $12/ton at the mine mouth and unit train transportation adds $6/ton for a typical 350 mile distance. The total $18/ton is equivalent to $\$0.80/10^6$ Btu for a coal with a heating value of 11,300 Btu/lb. The cost of Koppers Totzek 300 Btu gas using this coal would be $\$1.50/10^6$ Btu.

Economic evaluations included in Combustion Engineer's coal gasification program indicate LBG adds $\$0.45/10^6$ Btu to coal cost while MBG adds

Table 3-7. Summary of Operating Cost Estimates

PLANT NUMBER	A1-L	B1-L	C1-L	H1-L	A1-K	15-K
Nominal Plant Output MW	500	500	500	499	500	500
Net Plant Heat Rate	9,440	9,420	9,420	7,814	9,040	8,920
Number of Gas Turbines	-0-	-0-	-0-	3	-0-	-0-
Steam Throttle PSIG	2,520	2,520	2,520	2,520	2,520	2,520
SH DEGF	1,000	1,000	1,000	1,000	1,000	1,000
Reheat DEGF	1,000	1,000	1,000	1,000	1,000	1,000
Waste Heat FW Heater	-0-	1	-0-	3	-0-	-0-
Gross Plant Output MW	520	519	519	506.8	518	519
Auxiliary Power MW	17.4	16.4	16.4	5.2	15.4	16.4
Transformer Losses MW	2.6	2.6	2.6	2.6	2.6	2.6
Net Output MW	500	500	500	499	500	500
Annual Net Generation Million KWHR						
At 5000 Hr/Yr	2,500	2,500	2,500	2,495	2,500	2,500
At 7500 Hr/Yr	3,750	3,750	3,750	3,742	3,750	3,750
Capital Costs - $1000	125,947	125,771	122,101	116,786	121,344	121,491
Fuel Cost - $/Mil BTU	1.25	1.25	1.25	1.40	1.50	2.05
Annual Fixed Charges at 20%/Yr - $1000	25,189	25,154	24,420	23,357	24,269	24,298
Annual Operating and Maint. Labor - $1000	1,320	1,320	1,320	1,320	1,320	1,320
Annual Maintenance Mat, & Supplies - $1000						
At 5000 Hr/Yr	1,040	1,038	1,038	1,394	1,036	1,038
At 7500 Hr/Yr	1,560	1,557	1,557	2,091	1,554	1,557
Annual Fuel Cost - $1000						
At 5000 Hr/Yr	29,500	29,437	29,437	27,294	33,900	45,719
At 7500 Hr/Yr	44,250	44,156	44,156	40,941	50,850	68,572
Total Annual Operating Costs - $1000						
At 5000 Hr/Yr	57,049	56,950	56,216	53,365	60,525	72,371
At 7500 Hr/Yr	72,319	72,187	71,453	67,709	77,993	95,748
Energy Cost Mills/KWHR						
At 5000 Hr/Yr	22,820	22,780	22,486	21,389	24,210	28,948
At 7500 Hr/Yr	19,285	19,250	19,054	18,092	20,748	25,533

TABLE 3-8

ENERGY COST COMPUTATIONS

1. Net Plant Heat Rate $= \dfrac{\text{Total Fuel Fired}}{\text{Gross MW - Auxiliary Power}} = \dfrac{\text{Total Fuel Fired}}{\text{Net Plant MW}}$

2. Annual Net Generation = Net Plant MW x Hours

3. Maintenance Material and Supply Cost = Gross KWHRS/yr x Mills/KWHR Cost

4. Annual Fuel Cost = Annual Net Generation x Net Plant Heat Rate x Fuel ($\$/10^6$ BTU) Cost

5. Total Annual Operating Cost = Annual Capital Cost + Annual Fuel Cost + Annual Labor Cost + Annual Maintenance Materials

6. Unit Energy Cost $= \dfrac{\text{Total Annual Operating Costs}}{\text{Annual Net Generation}}$

$0.70/10^6 Btu (the same as the above estimates for MBG). Therefore, the total price used for Lurgi LBG is $1.25/10^6 Btu; for Koppers Totzek MBG, $1.50/10^6 Btu. This prices are for fuel delivered at low pressure (10 psig) and have been used for all systems except H1. Plant I5 needs 138.5 lbs oxygen per 10^6 Btu of fuel for combustion. At the 1974 U.S. average oxygen price of $8/ton, this adds $0.55/10^6 Btu to the MBG for a total price of $2.05/10^6 Btu.

It should be noted that the above prices are for fuel delivered at low pressure (10 psig). In the Lurgi gasification process, the fuel will be expanded from 132 psig through a turbine to 10 psig and this will yield more than enough power to drive the gasifier air compressors. However, if the gas is delivered at gasifier pressure, additional energy will be required to compress the air for the gasifier and the cost of the fuel will be correspondingly higher, $1.40/10^6 Btu for Lurgi LBG at 654°F and 132 psig compared to $1.25/10^6 Btu for the low pressure Lurgi systems. The annual fuel costs are the product of these rates, the net heat rates, and the annual hours of power generations (Item 4 of Table 3-8).

Annual operating and maintenance labor costs represent plant staffs of 78 people for each plant and are based on 1974 staff salary levels plus 35 percent administrative cost. Maintenance materials and supplies costs are based on 0.40 mills/kWh (gross) for the steam plans and 0.55 mills/kWh (gross) for the combined cycle plant. These represent composite total plant systems. Maintenance rates for the combined cycle plants are prorated according to the percentages of steam turbine and gas turbine outputs. The annual maintenance materials and supplies costs are the products of the composite plant rates, the gross plant outputs, and the hours per year (Item 3 of Table 3-8).

The total annual operating costs are the sums of the fixed charges and the fuel, labor and maintenance costs (Item 5 of Table 3-8). Unit energy costs are the total annual operating costs divided by the annual new power generation (Item 6 of Table 3-8). The resulting energy costs are the overall evaluation of plant cost and performance economics for comparison purposes, assuming the same plant location and power transmission costs.

The supercharged boiler combined cycle plant (H1-L) has the lowest overall energy costs, capital costs per kw, net heat rate and the lowest fuel costs.

The three other Lurgi LBG plants (A1-L, B1-L and C1-1) have nearly identical overall energy costs approximately 6 percent higher than Plant H1-L. Plant A1-L fired with Koppers Totzek fuel has overall energy costs approximately 16 percent higher than Plant H1-L; primarily due to the higher fuel cost and the use of oxygen in the boilers.

3.1.5 Heat Transfer Surface Requirements

The combustion chambers for each of the six systems were analyzed with Combustion Engineer's Lower Furnace Program described in Appendix B. This program has demonstrated good agreement with test data from tangentially-fired natural gas utility boilers, but has not been calibrated for other fuel gases. Although the precise numerical results obtained here cannot be verified with test data, they should be mutually consistent, allowing accurate comparison of the six systems.

The results for tangential firing are listed in Table 3-9. Although the Lower Furnace Model could not be directly applied to opposed wall firing, the results should be similar. A comparison of tangential and horizontal firing with natural gas based on Combustion Engineer's Engineering Standards showed that for the same heat inputs, furnace size, and burner location, the furnace outlet temperatures (and hence, waterwall absorptions) were nearly identical for the two firing modes. Unfortunately the very high gas recirculation for System I5 was well-beyond the range of C.E.'s Standards and comparison was impossible.

The results of the Lower Furnace Program (waterwall absorption, furnace outlet temperature, and net radiation flux from the furnace) provide the necessary inputs for determining the heat transfer surface requirements. A modified version of a C.E. surfacing program was prepared to handle LBG products. As with the Lower Furnace Program, a high degree of confidence in the results listed in Table 3-9 should be assumed for mutual comparison only.

Table 3-9. Summary of Heat Transfer Surface Requirements

System	A1-L	B1-L	C1-L	H1-L	A1-K	I5-K
Superheater (FT^2)	64,676	64,552	54,367	2,514 TOT*	52,693	48,585
Reheater (FT^2)	74,735	92,220	67,891	5,169 TOT	72,412	64,827
Economizer (FT^2)	439,833	247,690	317,742	243,573 TOT	243,690	77,290
Furnace & Backpass (FT^2)	34,354	30,452	31,871	19,227 TOT	30,452	29,492
Evaporator	-	-	-	-	-	-
Special Heaters						
Fuel Heaters (2)	252,800 TOT	97,500 TOT	-	-	-	233,108 TOT
O_2 Heaters (2)	-	-	-	-	-	169,430 TOT
Evap - SH (3)	-	-	-	45,200 TOT	-	-
Par. FW (2)	-	-	-	517,242 TOT	-	-

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* In cases where more than one unit was included in a classification such as superheater, TOT refers to the total surface area for all such units.

Material requirements for the furnace and boiler are generally similar to those of conventional steam power plants. Low temperature components such as the economizers coils are carbon steal with chrome-moly alloy steels for high temperature superheat and reheat tube assemblies. Burner nozzles are generally cast stainless steel. The boiler-combustors for system H1-L will contain a larger percentage of ferritic and stainless alloy steels due to the expected higher gas temperatures.

Each system was examined for additional components which may require special materials due to high temperature service. These components were found to be:

System	Component	Service
B1-L	Fuel Piping	Carries 1500°F gas @ 10 psig to Precooler
C1-L	Fuel Piping	Carries 1500°F gas @ 10 psig to Burners
C1-L	Burner Nozzles	Firing 1500°F gas
H1-L	Gas Pipe to Gas Turbine	Carries 2000°F gas

Material selections were made consistent with these requirements for the capital cost comparisons. To allow for uncertainty in the corrosive potential of the fuel, overly expensive materials were selected in some cases but the incurred increment in capital cost was not sufficient to decrease the accuracy of the comparisons.

3.1.6 Burner Designs

Full-load burner design parameters are presented in Table 3-10 for each of the systems. Tangential burner preliminary designs have been prepared for all systems except H1-L. These burners are of the gas spud type. Systems A1-L, B1-L, A1-K and I5-K utilize tilting burners for reheat steam temperature control and system C1-L has a fixed nozzle design, relying on gas recirculation

Table 3-10. Furnace Design for Burning Offgas from Coal Gasifiers — MCR Burner Design Parameters

	SYSTEM		A1-L	B1-L	C1-L	H1-L	A1-K	I5-K
	OXIDANT		AIR	AIR	AIR	AIR	AIR	OXYGEN
	GR THRU WBOX	%	10	10	10	0	15	205
	OVERFIRE AIR	%	0	15	15	0	0	0
	EXCESS AIR	%	15	15	15	15	15	5
FUEL TO BURNER	FIRED	10^6BTU/HR	4640	3990	3990	3650	4470	4380
	GROSS HEAT INPUT	10^6BTU/HR	4720	4310	4710	3899	4520	4598
	FLOW	LBM/HR	1,650,000	1,420,000	1,420,000	1,300,000	820,000	807,000
	TEMP.	^oF	451	750	1500	654	250	710
	PRESS.	PSIG	10	10	10	162	10	10
	DENSITY	LBM/FT^3	.0591	.0445	.0275	.5405	.0650	.0395
OXIDANT TO BURNER	FLOW	LBM/HR	3,340,000	2,870,000	2,870,000	2,626,000	2,970,00 0	611
	TEMP	^oF	384	487	487	671	460	392
GR TO BURNER	FLOW	LBM/HR	499,000	429,000	429,000	0	570,000	2,910,000
	TEMP.	^oF	511	543	543	-	523	784
MIXTURE TO BURNER	FLOW	LBM/HR	3,839,000	3,299,000	3,299,000	2,626,000	3,540,000	3,521,000
	TEMP.	^oF	400	493	493	671	467	731
	DENSITY	LBM/FT^3	.0461	.0417	.0417	.3533	.0432	.0393
	HEAT INPUT	10^6BTU/HR	304	335	335	381	337	631
FURNACE	NHP/PA	10^6BTU/HR-FT^2	1892.50	2.64	2.75	12.5 (Ea. of 3)	2.86	3.08
	WIDTH	FT	43.33	40	41	10.25	40	40
	DEPTH	FT	43.17	40	41	10.25	40	40

for steam temperature control. (Thermal expansion for this burner ruled out the possibility of tilt).

Preliminary opposed wall burner designs were also prepared for each system based on scaled-up Combustion Engineering Type R burners. Front and rear wall firing with three rows of four or five burners each was utilized for these systems. A single fixed vane (SV) burner mounted in the bottom of the furnace was employed in each of the System H1 boilers.

3.1.7 System NO_x Emission Assessment

Although the Combustion Engineering study was primarily directed toward the design and optimization of these systems from fuel utilization and economic viewpoints, NO_x emissions were also calculated.

Combustion Engineering's Lower Furnace Program described in Appendix B and reference 21 utilizes the axial temperature/time distribution of the combustor products generated by the basic program in combination with an NO formation rate based upon the Zeldovich mechanism. This program has been calibrated for both oil and natural gas firing and calculates NO_x emissions within ±15 percent for oil firing and ±10 percent for natural gas firing.

The burner designs described in the previous section were analyzed with this program and the results are presented in Figure 3-9 in relation to the maximum temperature in the furnace. Emissions were assumed to contain 5 percent of the total NO_x as NO_2. As expected, since the Zeldovich mechanism is very temperature sensitive, emissions rise dramatically with maximum temperature.

Although the Combustion Engineering program cannot be directly applied to the supercharged boiler*, it was applied to limit cases. The emissions for the supercharged boiler system shown in Figure 3-7 cover a 28-fold range. The minimum value is based on an atmospheric pressure boiler with the same

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*The NO_x subroutine is limited to atmosphere pressure calculations.

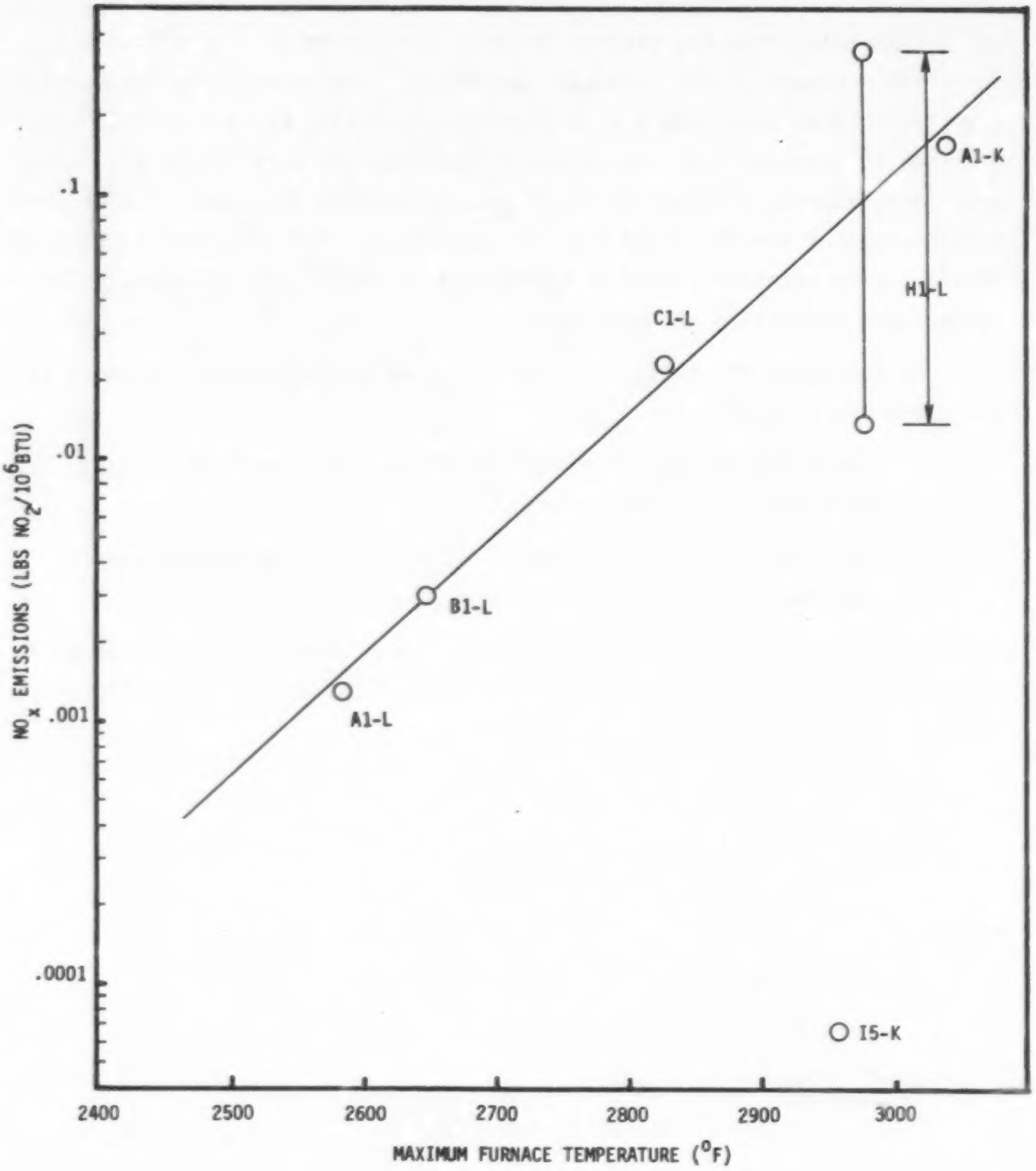

Figure 3-9. NO$_x$ Emissions Predicted by Combustion Engineering's Program for Tangential Firing

physical size and firing rate as the supercharged boiler. The maximum value was extrapolated from the minimum value by correcting for the effect of increased pressure in the Zeldovich mechanism. The basic lower furnace heat transfer program does have a high pressure capability and it was found that a change in pressure from one to ten atmospheres had very little effect on peak temperatures, although the exit gas temperature was lower at high pressure because of the increased overall absorption. The predicted temperature profiles were relatively flat at approximately 2900°F and consequently no temperature correction was necessary.

The increased NO_x emissions with increased pressure were estimated by evaluting the following two effects:

- The reaction rate is higher because of the increased partial pressure of the reactants.
- The furnace residence time is longer at high pressures due to radiant heat transfer requirements.

Habelt and Selker(21) assumed the ratio of the NO concentration produced in a cloud of combustion products of uniform composition to the NO concentration at equilibrium to be given by:

$$\frac{[NO]}{[NO]_{eq}} = 1 - e^{-C_1 t}$$

where:

t = residence time

$C_1 = 2K\,[N_2]\,[O]/[NO]_{eq}$

$K = 1.36 \times 10^{14}\, e^{-37943/T}$ cc/mol-sec
(reaction rate for $N_2 + O \rightarrow NO + N$)

T = temperature (°K)

They also assumed that for excess oxygen conditions $[NO]_{eq}$ is independent of pressure.

Applying these relationships to the pressurized boiler with a 1.0 second residence time at 10 atmsopheres and assuming equilibration of oxygen atoms, the pressure correction factor was calculated to be 28.

The results of this simplified analysis can be considered at best a rough approximation. Major questions regarding this procedure include:

- The lower furnace model is an empirical tool requiring "calibration" for different fuels and has not been used with LBG. It is also specific for corner-fired boilers.
- The Zeldovich mechanism assumption is difficult to justify, particularly if the majority of the NO_x is produced in the heat release zone because it neglects superequilibrium oxygen atom concentrations and Fenimore-type reactions.
- There is no mechanism to account for NO formation from fuel ammonia.

These limitations cast serious doubt on the accuracy of the C.E. computer model applied to pressurized combustors firing LBG. Section 4 discusses the application of a modular kinetic model to calculate limit-case emissions based on the best available kinetic mechanisms.

3.2 Integrated Gasifier/Power Plant Analysis

The comparative analysis in Section 3.1 demonstrated that subject to the limitations of existing technology and a separate gasifier, the best alternative (of those examined) was a combined gas and steam (COGAS) cycle power plant. In particular, the COGAS system had:

- Lowest heat rate (highest efficiency)
- Lowest capital cost
- Lowest annual fuel cost
- Lowest net energy conversion cost (mils/kWh)

This section extends the analysis of COGAS systems to integrated gasifier/power plants where heat and mass transfer in addition to fuel transfer couple the two units. The purpose is to provide some general background comments pertaining to thermodynamic cycle studies of gasifier-combined cycle systems and to suggest a general methodology for further systems studies. An overview of COGAS systems is first presented summarizing some of the important design variables and how they affect overall performance. The discussion then focuses on gasifier design and losses and the trade-offs between a supplementary-fired waste heat recovery boiler and a supercharged boiler, two factors which strongly influence combustor requirements. Finally, descriptions of six general classes of combustion devices which are most likely to evolve in the course of gasifier-combined cycle plant development are given.

3.2.1 An Overview of COGAS System Efficiency

The principal losses contributing to inefficiency in a coal gassification-combined cycle power plant are: the condenser heat rejection; the combustion product latent and sensible heat emitted through the exhaust stack; and any heat loss associated with the gassification product cooling. Other less significant losses are: heat transfer between various hot elements of the system and the surroundings; exhaust stream energy emissions from auxiliary equipment; and by-product streams containing combustibles, e.g., the tar-like residue from the coal gasification process which may be emitted as a waste stream or returned to the gasifier.

The efficiency of a coal gasification-combined cycle power plant can be defined by:

$$\text{Efficiency} = \frac{\text{Net Electrical Energy Output}}{\text{Higher Heating Value of Input Coal}}$$

This in turn can be expressed in terms of the system losses as:

$$\text{Efficiency} = 1 - \frac{\text{Losses}}{\text{HHV of Coal}}$$

where losses include all energy outflow fluxes from the system except electrical energy and the heat content of the coal is the only energy input to the system*. The basic concept of combined cycle systems is to cut these losses by effectively utilizing the high temperature turbine exhaust gases in a Rankine cycle to raise steam. The high turbine exhaust loss is thus replaced by condenser and boiler stack losses which combine to yield a lower total loss. Variations on this theme come about when the turbine exhaust temperature is too low (due to low turbine inlet temperature) to permit an efficient Rankine cycle. This low steam temperature and excess of available low grade energy from the exhaust which cannot be utilized in an economizer leads to high stack temperatures. Although the latter situation may be improved somewhat by incorporating a second low pressure steam cycle in the steam generator, a more effective approach is to improve the "quality" of the turbine exhaust by supplementary firing the turbine exhaust boiler, thereby raising its temperature. Once the efficiency of the steam cycle has been sufficiently improved, any further supplementary firing serves only to bias the combined cycle towards a pure Rankine cycle, and hence, to lower the overall efficiency.

Provided the exhaust energy can be used effectively, the key to enhanced efficiency is to increase the fraction of fuel energy extracted by the gas turbine. This decreases the turbine exhaust energy, a large portion of which is necessarily lost through the condenser and stack. Higher gas turbine efficiency is accomplished through increased turbine inlet temperature. In the idealized Brayton cycle, efficiency is a function of compressor pressure ratio only and is independent of turbine inlet temperature. However, due to inefficiencies in both the compression and expansion processes the relationship between the temperature increase due to combustion and the temperature rise associated with compression becomes an important factor. High compression ratios are permissible only with a high degree of energy addition in the combustor which, in turn, leads to high turbine inlet temperature. High inlet temperatures also lead to high exhaust temperatures, and hence, to more effective Rankine cycle waste energy recovery systems. For low turbine inlet temperature, optimum compression ratios for COGAS systems are somewhat lower than for stand-alone gas turbines due to the trade-off between gas turbines and waste heat recovery efficiencies. Similarly, establishing optimum gas turbine reheat and recuperation requires consideration of the complete COGAS system. This is discussed further in later sections.

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*Any electrical input to the plant is combined with the generator output to form the net and any auxiliary heating is combined with the HHV of the coal.

An alternative to supplementary firing the exhaust boiler and a more effective approach to improving the utilization of turbine waste heat is the integration of a supercharged boiler with the gas turbine combustor. Here the supplementary fuel addition is upstream of the turbine rather than downstream in the waste heat recovery boiler. Again sufficient steam raising (boiling and superheating) is accomplished through additional firing of the gas turbine combustor (supercharged boiler) to allow full utilization of the turbine exhaust for feedwater heating. The greater effectiveness of the supercharged boiler is a result of the greater mass and energy flow through the gas turbine, and hence, greater turbine power extraction than for a fired waste heat boiler.

Attempts to optimize net plant heat rate and define combustion devices on the basis of separate studies of the gasifier and combined cycle plant (treating the fuel as "coming over the fence") have inherent difficulties and the results must be examined with considerable caution. This applies equally to pollution potential, plant efficiency and cost benefit trade-off studies. The results of these optimization attempts do not consider the interaction of gasifier and power plan so that optimizing one unit could degrade the performance of the other. The gasifier and combined cycle systems can be intimately coupled through several heat and mass transfers and trade-offs:

- Heat exchange between the gasifier's raw gas (prior to H_2S removal) and the boiler feedwater
- Gasifier and gas turbine compressor requirements
- Gasifier and gas turbine combustor pressure losses
- Fuel gas temperature and composition

The next section describes the effects of some of these variables on overall system performance and demonstrates that the effectiveness of the gasifier depends greatly on the manner in which it is matched to the combined cycle. Thus, it is impossible to define a meaningful gasifier efficiency without examining the coupled system. The following section examines the trade-offs between a supplementary-fired waste heat recovery boiler and supercharged boiler as system design parameters vary.

3.2.2 Gasifier Losses

The coal gasification process yields a product which is lower in both total energy and available energy than the total energy input. It is convenient to classify the energy losses as either "irretrievable" or "potential". Irretrievable losses are those gasifier energy losses which cannot be utilized by the power plant. Examples include:

- Water or steam added to the gasifier
- Carbon loss in ash
- Residual tars not returned for combustion or gasification
- Gasifier heat losses to the environment

Potential losses are those gasifier energy losses which could be utilized by the power plant depending upon power plant design. Two important examples include:

- Sensible heat in the fuel gas
- Work of air compression

It is difficult to speak of gasifier efficiency or losses independently since the gasifier and combined cycle plant are so closely coupled. However, a useful figure-of-merit or efficiency for the gasifier portion of such a system can be defined as the ratio of the net power plant efficiencies for a gasifier-combined cycle system to the corresponding efficiency of a similar combined cycle system burning coal directly (ignoring the design problems and the energy penalties associated with corrosion suppression and particulate and sulfur cleanup). For example, if a gasifier could be operated with losses equal to those incurred burning coal directly, then it would have 100 percent efficiency under this definition. Any degradation in plant performance from this ideal situation is assigned as gasifier inefficiency.

Using this definition, a typical one-atmosphere gasifier feeding a conventional boiler (with or without precooling and feedwater heat exchange) will have an efficiency of approximately 83 percent which corresponds to the irretrievable losses cited above. A system mismatch, such as a high pressure gasifier in conjunction with a combined cycle employing a low temperature gas turbine feeding a fired exhaust boiler, will yield efficiencies on the order of 73 percent. The additional 10 percent loss is due to throttling the major portion of the fuel gas prior to entering the fired exhaust boiler. Another example of mismatch is employing gasifier intercooling for feedwater heating in an unfired turbine exhaust waste heat boiler. This not only diminishes the turbine power but is especially ineffective because of the overabundance of low temperature heat already available. Here the gasifier efficiency may be on the order of 78 percent. On the other hand, a well-optimized gasifier-COGAS system should be able to operate with 90 percent gasifier efficiency corresponding to the minimum irretrievable losses.

3.2.2.1 Water Content – Irretrievable Loss

LBG and its products of combustion contain more water than the products of combustion of coal. This is due to the introduction of steam in the gasification process which provides hydrogen donation via the water/gas reaction. In the air-blown Lurgi process the steam addition rate is approximately one pound of steam per pound of coal. Roughly 50 percent of this water appears as water vapor in the LBG (which is knocked out if the gas is quenched) and eventually all of it appears as additional water vapor in the final products of combustion leaving the power plant stack. In either case its latent heat is lost and the lower heating value (LHV) of the fuel is thus diminished. In a conventional boiler burning a typical Lurgi gas the efficiency is degraded by approximately 10 percent which corresponds to the full reduction of the lower heating value due to the presence of additional water vapor. This conclusion is independent of gasifier intercooling. However, if the LBG is fired in a gas turbine the additional water vapor adds to the working fluid passing through the gas turbine much as in a Rankine cycle. That is, the expenditure of the latent heat in the process of creating the vapor provides the turbine with a high pressure gaseous working fluid without the penalty of compressor energy. Although the vapor is raised to high temperature in the gas turbine it is not expanded over the very large pressure ratio of a Rankine cycle, and hence, the incremental efficiency associated with the water vapor working fluid is not up to typical steam cycle efficiency. In a typical COGAS system employing an unfired waste heat boiler the incremental efficiency associated with the additional water vapor is approximately 30 percent[*]. This is less than the overall cycle efficiency, and hence, represents a degradation in performance. The effective gasifier efficiency is down by 5 percent, or approximately one-half of the penalty associated with burning the LBG in a conventional boiler. In the COGAS system, as gasifier water injection increases, the gas turbine power fraction and the fuel/air ratio both increase while the turbine exhaust sensible heat, the steam-side power, and the condenser heat loss all decrease more than with the conventional boiler, thus verifying the net advantage of the COGAS system.

The supercharged boiler COGAS system has the same advantage indicated above for the waste heat boiler. Supplementary-fired waste heat boilers and fully-fired exhaust boilers suffer the same losses as conventional boilers, but to a lesser degree.

3.2.2.2 Other Irretrievable Losses

Intercooling the gasifier product knocks out approximately 50 percent of the injected water and eliminates this portion of the water vapor as an effective gas turbine working fluid. In this instance the effective gasifier efficiency is reduced approximately 7½ percent due to water injection when coupled with supercharged or waste heat boiler COGAS systems. Thus the effect of intercooling just due to the water vapor effect alone is roughly one point in overall system efficiency.

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[*] That is, when additional fuel is burned to raise steam which is injected into the gasifier, 30 percent of that fuel energy is converted into work.

Losses associated with heat loss to the environment, carbon loss in the ash, and residual tarts which are not returned for combustion as part of the gasification process amount to typically 7-8 percent. This loss is probably reducible to 5 percent with an optimum design.

3.2.2.3 Sensible Heat — Potential Loss

Typical LBG raw product gases leave the gasifier with sensible heat equivalent to 10-15 percent of the heat of combustion of the coal input. For pressurized systems, typically one-third of this can be associated with the increase in energy resulting from combustion air compression. Some or all of the sensible heat can be effectively used by the COGAS system depending upon: the system integration of gasifier and power plant; the need for cold H_2S cleanup; and the combined cycle characteristics. In one extreme the sensible heat may be dumped overboard in a quench process or it may be used for industrial processes which require low quality heat. In the other extreme, the raw gas may pass through a hot cleanup process (if available) and into a combined cycle system with undiminished temperature in such a manner as to utilize all of the sensible heat effectively. Alternately, if an unpressurized gasifier is used to feed a conventional boiler, all of the sensible heat can be effectively utilized through a heat exchange with the feedwater prior to cold cleanup and no losses are incurred. In between these extremes are situations in which partial recovery is accomplished through a somewhat ineffectual exchange of heat between raw gasifier products (prior to cold cleanup) and various portions of the COGAS cycle.

A rough rule describing the cumulative effects of intercooling is that it becomes more significant as turbine inlet temperature increases. There are three potential effects of gasifier intercooling on performance:

- Loss of high pressure gaseous working fluid (water vapor) through condensation.
- Reduction of gas turbine power fraction through decrease in turbine energy throughput.
- Inability to effectively utilize low grade heat from intercooler in feedwater heating or steam raising.

The first effect was discussed in the last section and represents typically one point in performance for supercharged and waste heat boiler systems. The second effect is of little importance in low excess air supercharged and low excess air exhaust-fired systems because the turbine energy throughput is essentially unaltered. In these cases the reduction of fuel enthalpy is manifested in a reduction of heat input to the supercharged or exhaust-fired boilers. This loss is retrieved by feedwater heating and boiling from the intercooler. However, for high excess air systems this effect can be appreciable because turbine energy throughout is substantially affected by fuel intercooling. The effect can be several points in system efficiency.

Finally, the third effect can be significant for COGAS systems with moderate turbine inlet temperature (2000°F) incorporating high excess air boilers (supercharged or exhaust). In these systems there is an overabundance of low quality exhaust heat for feedwater heating and boiling which makes it impossible to effectively utilize the intercooler heat. The effect becomes less significant for high turbine inlet temperature waste heat systems and is nonexistent for low inlet temperature systems which employ low excess air combustors. The latter have a sufficiently large quantity of high quality heat input that they can effectively utilize the lower temperature intercooler heat for feedwater heating.

3.2.2.4 Work of Air Compression - Potential Loss

Compression is manifested as an increase in enthalpy of the raw gas product as well as an increase in its available energy. It is recovered in part in any thermodynamic cycle which converts heat to work. However, if a pressurized gasifier is utilized for a one-atmosphere conventional boiler only about 35 percent of this energy will be recovered. The net effect is a loss of mechanical energy equal to approximately 3 percent of the heat of combustion of coal which is equivalent to a 9 percent reduction in gasifier efficiency.

3.2.3 Supercharged Versus Fired Exhaust Boilers

If a conventional steam plant is fired with LBG from a one-atmosphere gasifier there is approximately a 17 percent degradation of net heat rate over direct coal firing. This leads to an overall gasifier-steam plant efficiency of roughly 32 percent using state-of-the-art technology. This conclusion is independent of whether the raw gasification product is uncooled or fired in the boiler at a high temperature because only low quality (i.e., low temperature) heat is required in a conventional boiler; there is no need for heat input at the high peak temperature associated with combustion. The usual boiler heat transfer process is over a large temperature differential giving rise to high entropy production (irreversibility).

The utilization of the high temperature of combustion in a gas turbine topping cycle is the key reason for increased performance in a COGAS cycle. The waste heat from the gas turbine exhaust is used as the heat input to a conventional steam turbine bottoming cycle.

Depending upon overall cycle design, the heat in the gas turbine exhaust may or may not have sufficient temperature for an optimum steam bottoming cycle. If the temperature is too low, it can be raised either by burning more fuel in the gas turbine combustor and transferring the heat to the steam cycle (supercharged boiler) or by bringing more fuel directly in the turbine exhaust (supplementary firing). The supercharged boiler is the preferred COGAS system for use with LBG for turbine inlet temperatures up to levels well in excess of 2000°F. The precise inlet temperature at which the unfired waste heat boiler system becomes superior has not yet been determined, but it may be as high as 2400°F. In this high temperature regime the supercharged boiler would be fired with high excess air.

The principal reasons for the thermodynamic superiority of a supercharged boiler over a fired exhaust boiler include:

- It allows the system to take advantage of additional water vapor in the combustion products due to gasifier steam injection.
- It allows higher gas turbine energy throughput, and hence, higher turbine fractional power due to increased mass flow through the turbine.

- Due to its high operating temperature, it more effectively serves the basic purpose of providing high quality energy input for steam raising which, in turn, allows the effective utilization of the low quality turbine exhaust energy.

The cumulative effects lead to advantages which decrease as turbine inlet temperature increases. At low turbine inlet temperatures the improvement can amount to several percentage points in overall system efficiency. The utilization of water vapor dominates the other advantages, and hence, the attractiveness of supercharged boilers over fired exhaust boilers is predominantly a consequence of firing LBG -- a factor generally ignored in most studies.

3.2.3.1 Low Turbine Inlet Temperature Combined Cycle Systems

Figure 3-10a shows a typical design for a counterflow unfired waste heat boiler where the turbine exhaust gases first encounter the superheat section, then the evaporator sections and finally the economizer. Figure 3-10b shows the gas and steam side temperature distribution for a typical low turbine inlet temperature case and illustrates two important and related points. First the quality of the steam generated is poor with an attendant low steam-side efficiency. Secondly, the "pinch point" constraint forces a high gas stack temperature*. There is, of course, a trade-off between attainable steam quality and stack losses, and both of these factors are related to turbine exhaust temperature. When the exhaust temperature becomes sufficiently high that an efficient steam cycle can be operated off the waste heat without excessive stack losses, then there is no need for supplementary firing. For temperatures below this critical value supplementary firing is required to bring up the steam-side efficiency and minimize stack losses. This supplementary firing can occur either in the gas turbine combustor (i.e., a supercharged boiler) or in the waste heat boiler.

For turbine inlet temperatures of 2000°F and below there is a clear advantage to the supercharged boiler fired by a pressurized gasifier. The

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*There is an excess of low quality heat which is unusable.

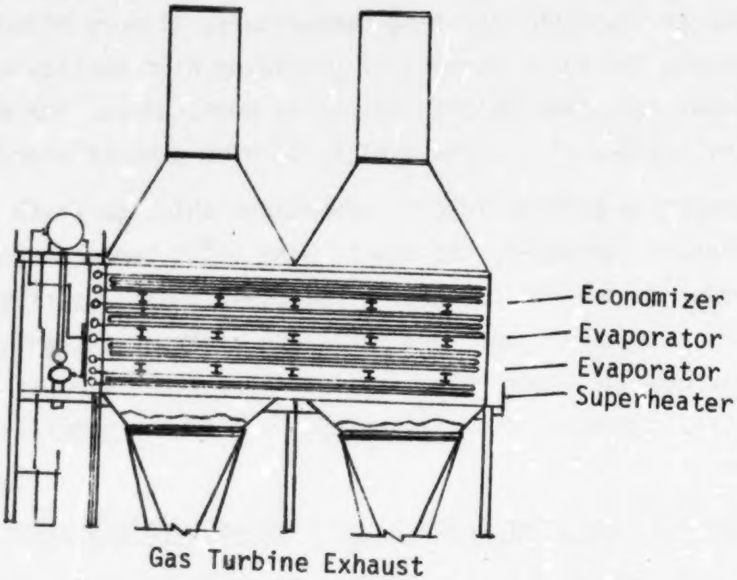
Economizer
Evaporator
Evaporator
Superheater
Gas Turbine Exhaust

Figure 3-10a. Unfired Steam Generator Design

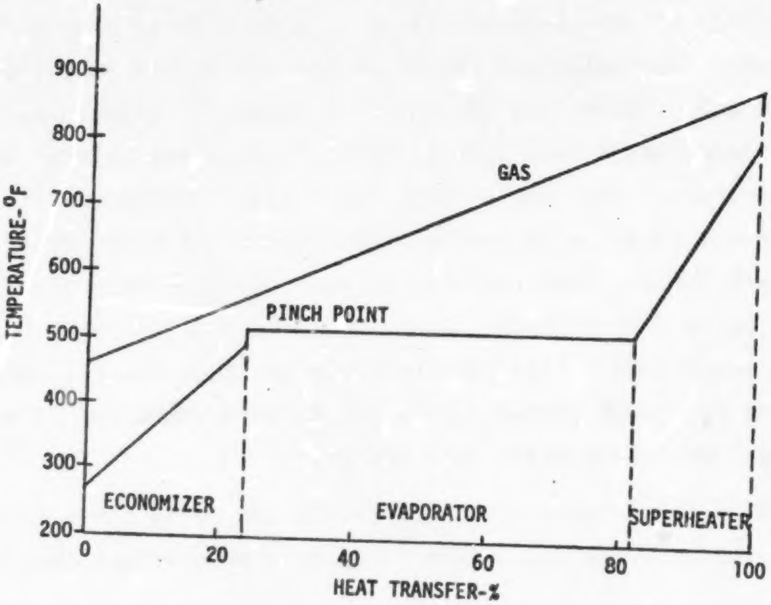

Figure 3-10b. Typical Gas and Steam Temperatures Unfired Steam Generator

advantage lies primarily in the higher fraction of system power delivered by the gas turbine while the steam-side efficiency remains the same for both systems. The low excess air supercharged boiler, typical of low turbine inlet temperature systems, fully utilizes the gas turbine exhaust heat for feedwater heating, and hence, the boiler stack losses are low. Further, the condenser losses on the steam-side are lower for the supercharged boiler case because of the lower fractional steam-side power. The higher fractional gas turbine power for the supercharged boiler is due to the higher energy flow through the turbine under these conditions.

Assuming the fired exhaust boiler is fed by a separate one-atmosphere gasifier, then the supercharged system has roughly a three percentage point advantage in overall system efficiency over the exhaust-fired boiler. The advantage becomes substantially greater if the same high pressure gasifier feeds both the gas turbine and exhaust boiler as is sometimes assumed in making the comparison. Overall gasifier-COGAS efficiency for these low turbine inlet temperature systems can reach approximately 37 percent. If gasifier intercooling is employed, then 36 percent efficiency can be achieved at 2000°F.

3.2.3.2 Moderate Turbine Inlet Temperature Combined Cycle Systems

Most attention to date has been given to supercharged boilers and furnace-fired exhaust boilers under the low excess air conditions which are optimum for low turbine inlet temperatures. However, as turbine temperature increases, the amount of supplementary firing required to bring the system to optimum performance decreases with an attendant increase in excess air. Excessive supplementary firing does little to enhance the steam-side efficiency while it increases the steam-side fractional power, and hence, reduces overall efficiency. The incremental efficiency associated with excessive supplementary firing (that is, the efficiency of conversion of the incremental addition of fuel) at 2200°F turbine inlet temperature is on the order of 37 percent for the exhaust boiler and 38½ percent for the supercharged boiler. These figures are high in comparison to a conventional Rankine cycle considering the gasifier losses. This is a consequence of the low incremental change in stack losses due to the decreasing excess air. The overall cycle efficiency is greater than 40 percent for the optimum supercharged boiler with 2200°F turbine temperature, and hence, excessive supplementary firing degrades the system performance.

Figure 3-11 illustrates qualitatively how the supercharged boiler COGAS system efficiency depends on excess air and turbine inlet temperature. For low turbine inlet temperatures the performance increases with decreasing excess air until the minimum excess air line for satisfactory combustion is reached. As inlet temperatures increase the optimum excess air level becomes greater than the minimum line. To the left of this optimum point (that is, at lower excess air) the system performance increases with increasing excess air. The curve marked ($\approx 2000^{0}$F) shows equal system performance for the minimum excess air supercharged boiler and the gas turbine-waste heat boiler. This result is often misinterpreted as meaning that for turbine temperature above 2000^{0}F it is no longer desirable to use a supercharged boiler. As can be seen from the figure, this is not the case. Under optimum excess air conditions the supercharged boiler appears to be attractive for turbine temperatures well above 2000^{0}F. The actual turbine temperature for which the supercharged boiler is no longer attractive, and for which performance increases monotomically with increasing excess air, has not been established at this time.

3.2.3.3 High Turbine Inlet Temperature Combined Cycle Systems

Again referring to Figure 3-11, as turbine inlet temperature climbs, a point is eventually reached where the steam cycle receiving heat from an unfired waste heat boiler is sufficiently efficient that any supplementary firing will not improve steam cycle performance but will degrade overall performance by reducing the gas turbine power fraction. The optimum waste heat boiler COGAS systems have efficiencies which can reach 50 percent with turbine inlet temperatures of 2800^{0}F. Gasifier intercooling would degrade this efficiency by several percentage points.

3.2.4 Generalized Approach to Cycle Analysis

The preceding discussion demonstrated that the influence of system design and operational variables on combustor requirements is subtle and easily defies intuition. A particular danger in such an analysis is the omission of sufficient generality of concepts and attention to detail in the approach. For example, if the analysis above had been restricted to unfired waste heat boilers or low excess air supercharged boilers, an entire class

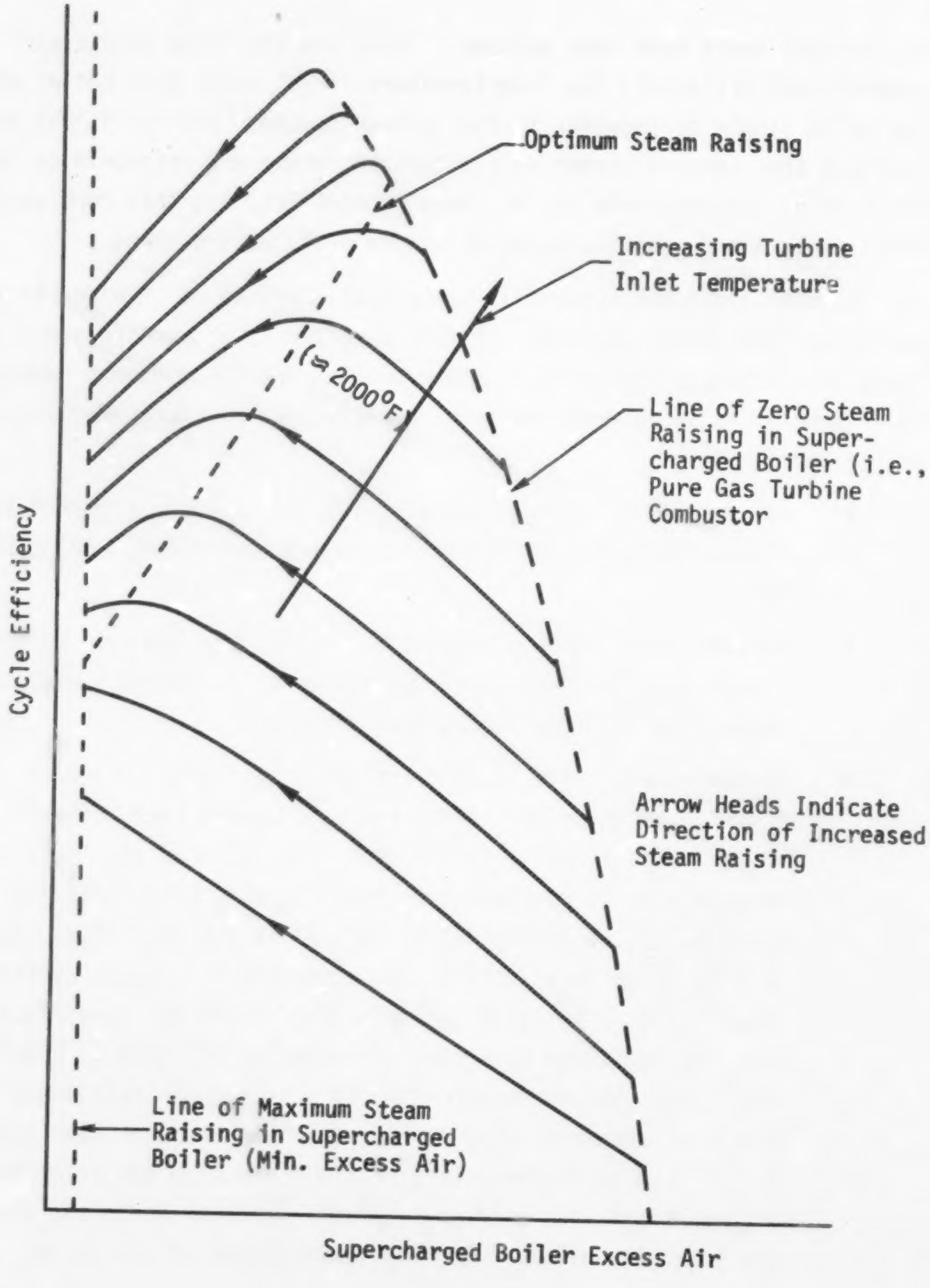

Figure 3-11. Supercharged Boiler Combined Cycle Efficiency as a Function of Excess Air

of concepts would have been omitted. These are the "high excess air" supercharged boiler and the "supplementary-fired" waste heat boiler which may exist singly or together in the optimum system. Similarly, one might conclude that several stages of gas turbine reheat are desirable on the basis of no pressure drop in the reheat combustors, but this conclusion might prove wrong upon inclusion of a more detailed treatment.

A generalized and systematic analytical approach is required to properly define optimum combustors under various combined-cycle constraints. Six basic types of combustors should be considered. The four most common combustors are shown schematically in combined-cycle application in Figure 3-12 and are described below.

- Adiabatic Gas Turbine Combustor (Figure 3-12a). Figure 3-13 shows a Brown Boveri design for an industrial gas turbine firing LBG.
- Furnace-Fired Turbine Exhaust Boiler (Figure 3-12b). This is essentially a conventional LBG boiler which receives vitiated combustion air from the turbine exhaust.
- Supplementary-Fired Turbine Exhaust Boiler (Figure 3-12c). In order to increase the effectiveness of waste heat boilers it may be cost-effective for systems with moderate turbine inlet temperatures to supplementary fire a combustor located just upstream of the waste heat boiler. This combustor uses only a portion of the available oxygen contained in the gas turbine exhaust and is designed to limit the maximum gas temperature entering the steam generator to approximately 1200 to 1300°F. This allows the steam generator to maintain its relatively simple arrangement shown in Figure 3-10. The combustor must be designed to handle high excess air and high gas velocities without flame instability. With conventional fuels the burners are located directly in the duct work ahead of the boiler.
- Supercharged Boiler (Figure 3-12d). This is the system which has received considerable attention in the course of the present investigation.

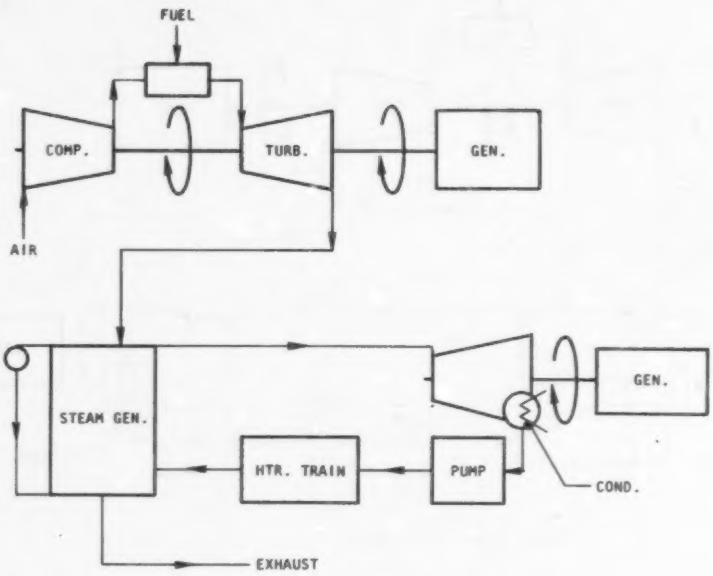
FUEL
COMP.
TURB.
GEN.
AIR
STEAM GEN.
GEN.
HTR. TRAIN
PUMP
COND.
EXHAUST

Figure 3-12a. Gas Turbine Plus Unfired Steam Generator

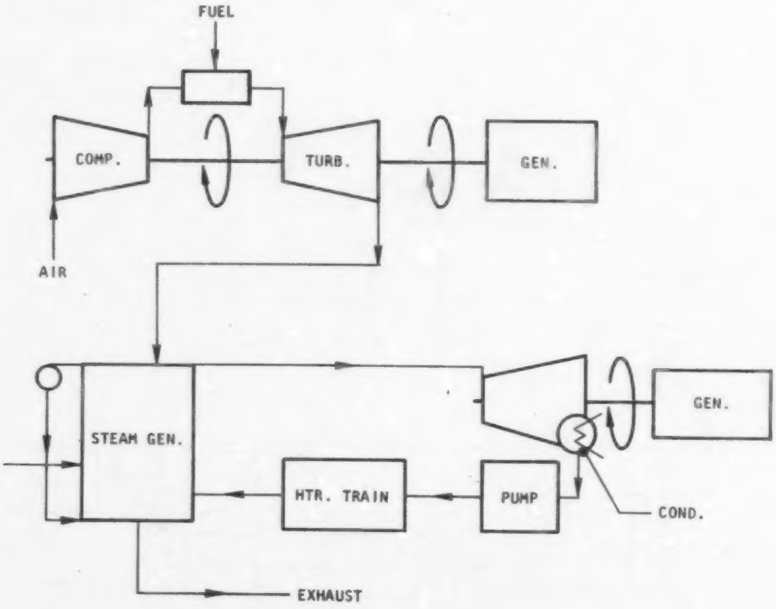
FUEL
COMP.
TURB.
GEN.
AIR
STEAM GEN.
GEN.
HTR. TRAIN
PUMP
COND.
EXHAUST

Figure 3-12b. Gas Turbine Plus Furnace-Fired Steam Generator

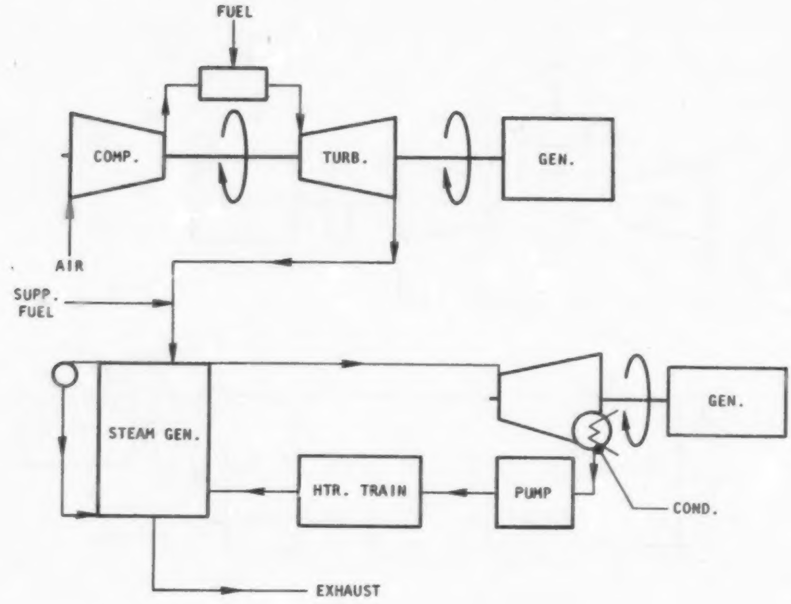
FUEL
COMP.
TURB.
GEN.
AIR
SUPP.
FUEL
STEAM GEN.
GEN.
HTR. TRAIN
PUMP
COND.
EXHAUST

Figure 3-12c. Gas Turbine Plus Supplementary-Fired Steam Generator

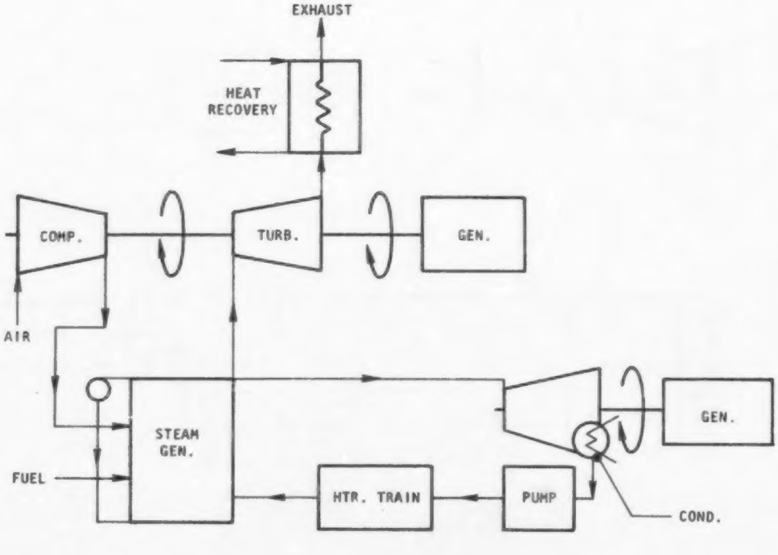
EXHAUST
HEAT
RECOVERY
COMP.
TURB.
GEN.
AIR
STEAM
GEN.
GEN.
FUEL
HTR. TRAIN
PUMP
COND.

Figure 3-12d. Supercharged Furnace-Fired Steam Generator Plus Gas Turbine

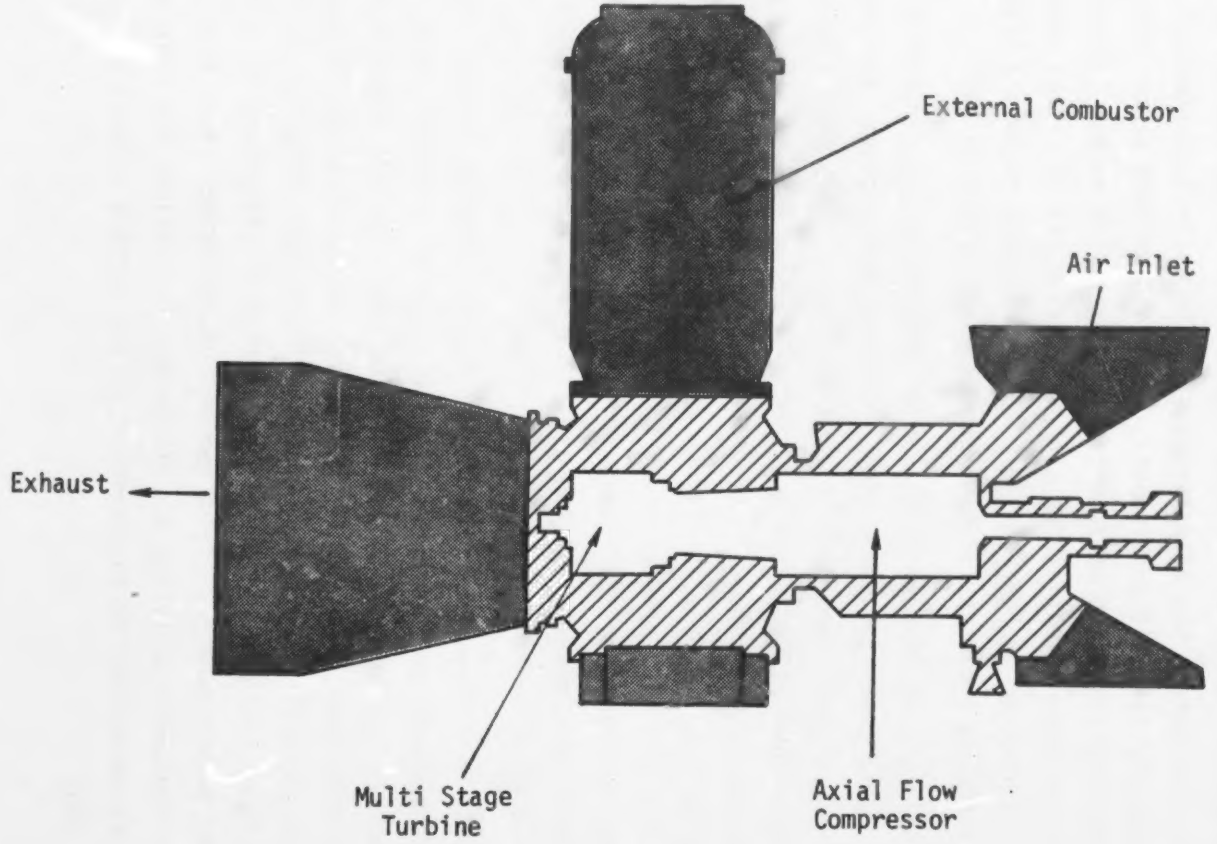
External Combustor
Air Inlet
Exhaust
Multi Stage Turbine
Axial Flow Compressor

Figure 3-13. Brown Boveri Industrial Gas Turbine with External Combustor

In addition to the four combustor types indicated above there are two more which deserve attention. These are shown schematically in combined-cycle application in Figure 3-14 and are described below.

- Gas Turbine Reheat Combustors (Figure 3-14). There is a cycle advantage to interstage reheating in the gas turbine portion of the cycle. The increase in turbine power fraction can be very substantial, while at the same time increasing the exhaust temperature, and hence, the effectiveness of the waste heat recovery. The excess air level is continuously decreased as more stages are added. Particular attention must be given to excessive reheat combustor pressure drop in optimizing such a system. Use of reheat combustors is referred to as "carnotizing" the gas turbine cycle and their use in combined cycle application should prove effective.

- MHD Combustors (Figure 3-14). MHD combined cycles fired with LBG offer the potential for a high efficiency power plant, and hence, the associated combustors deserve attention. Very high combustion temperatures (5000°F) are required which implies a high degree of recouperation as shown in Figure 3-14. An "interstage" recouperator followed by a conventional low pressure turbine stage is shown. This allows high temperature recouperation which could not be obtained otherwise. NO_x control via post-flame reduction and hold-up in the recouperation and waste heat boilers are possibilities to be investigated.

Figure 3-14 also shows the flow diagram for a suggested generalized cycle analysis computer program where all six types of combustors are potential elements in the system. Optimization would include the selection of the appropriate combustor type for a given set of constraints (e.g., turbine inlet temperature). Trade-off studies of pollutant potential versus systems efficiency could be conducted with parametric variations of combustor excess air and temperature around the optimum design point. Both high pressure and one-atmosphere gasifiers are included. This allows the possibility of feeding a furnace-fired or supplementary-fired turbine exhaust boiler with low pressure LBG.

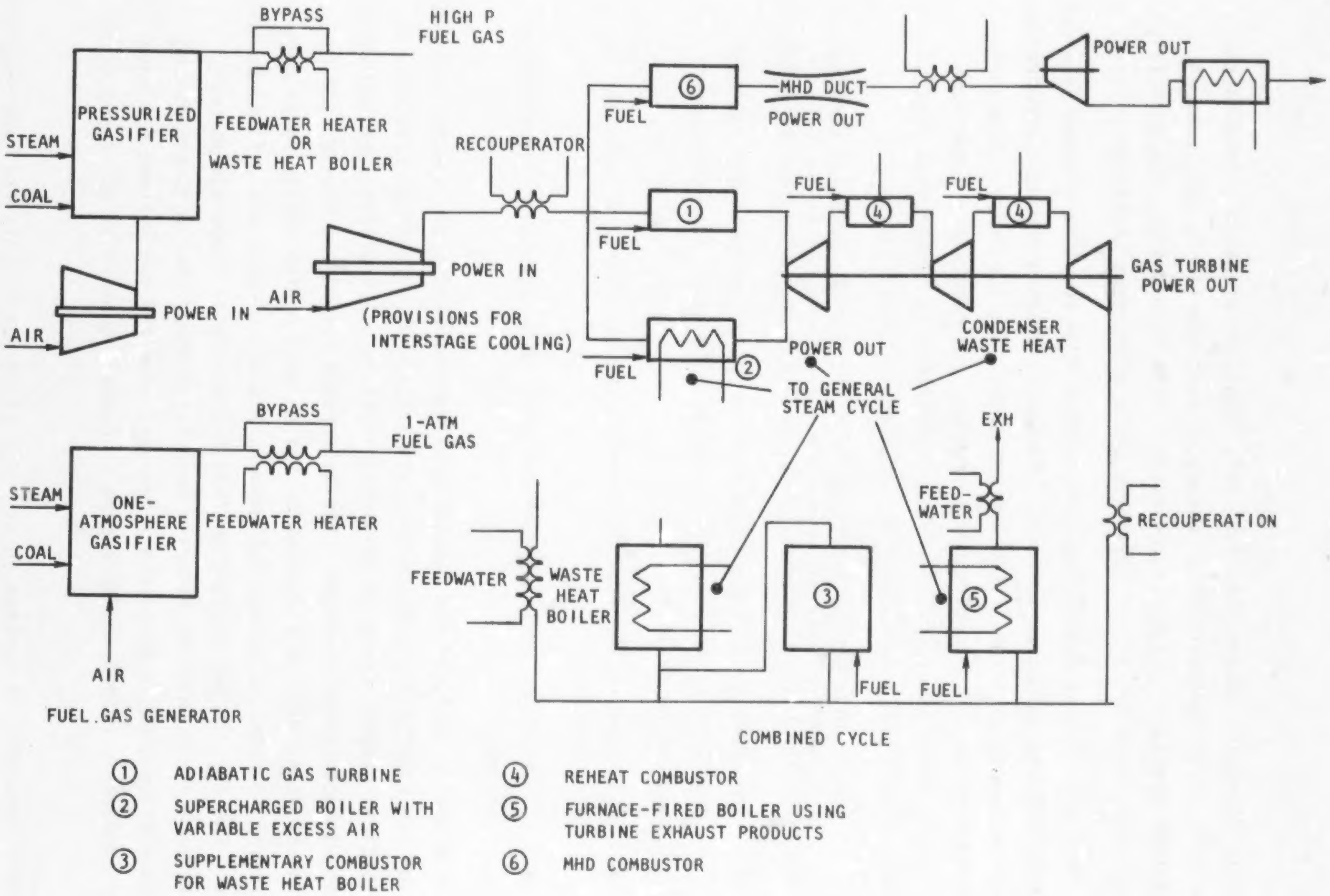
BYPASS
HIGH P FUEL GAS
PRESSURIZED GASIFIER
STEAM
COAL
FEEDWATER HEATER OR WASTE HEAT BOILER
AIR
POWER IN
RECOUPERATOR
AIR
POWER IN
(PROVISIONS FOR INTERSTAGE COOLING)
FUEL
⑥
MHD DUCT
POWER OUT
POWER OUT
FUEL
①
FUEL
④
FUEL
④
GAS TURBINE POWER OUT
FUEL
②
POWER OUT
CONDENSER WASTE HEAT
TO GENERAL STEAM CYCLE
BYPASS
1-ATM FUEL GAS
STEAM
ONE-ATMOSPHERE GASIFIER
COAL
FEEDWATER HEATER
AIR
FUEL GAS GENERATOR
EXH
FEED-WATER
RECOUPERATION
FEEDWATER
WASTE HEAT BOILER
③
⑤
FUEL
FUEL
COMBINED CYCLE
① ADIABATIC GAS TURBINE
② SUPERCHARGED BOILER WITH VARIABLE EXCESS AIR
③ SUPPLEMENTARY COMBUSTOR FOR WASTE HEAT BOILER
④ REHEAT COMBUSTOR
⑤ FURNACE-FIRED BOILER USING TURBINE EXHAUST PRODUCTS
⑥ MHD COMBUSTOR

Figure 3-14. Generalized Thermodynamic Cycle Analysis Flow Diagram

The flowchart labels the "fuel in", "gasifier steam in", "compressor power in", "turbine power out", "condenser heat ejection", and "exhaust stack heat ejection" points in the cycle. This information, appropriately manipulated, provides all of the gross cycle efficiency characteristics.

Much significant detail has been omitted from the flow diagram in order to emphasize the principle features. Feedwater heating through regeneration, economizers, and gasifier precooling are shown only implicity. Similarly, steam side reheat, gas turbine recouperation, and compressor interstage cooling are not shown in detail. Such refinement as desuperheat control are not shown at all, but should be included in the analysis.

3.3 Conclusions and Combustor Definitions for NO_x Emission Studies

Based on the results of this study, several conclusions can be drawn.

- The COGAS cycle firing LBG from an integrated gasifier has high potential efficiency when compared with other advanced power generating systems.
- Intercooling the fuel gas between the gasifier and combustor is undesirable.
- Supercharged boilers offer distinct advantages over fired exhaust boilers.

A properly designed and coupled gasifier-combined cycle system with sulfur removal can potentially achieve fuel utilization 90 percent as effective as the hypothetical direct firing of pulverized coal in a comparable combined cycle system without sulfur recovery. The integrated gasifier-combustor can be thought of as a multistage combustion system with a rich gasifying primary incorporating water injection followed by hot H_2S cleanup and a final burnout stage. Further, if one speculates that turbine inlet temperatures under direct coal firing will necessarily have to be lower than with LBG firing due to difficulties in particulate removal, then the two systems may have fully comparable overall efficiencies*. Overall conversion efficiencies of gasifier-combined cycle systems of 40 percent or greater can potentially be achieved with turbine inlet temperature of 2200°F and potential efficiencies approaching 50 percent are attainable as turbine inlet temperatures climb to 2800°F.

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*A 200°F reduction in turbine inlet temperature has roughly the same impact as the gasifier losses. This comparison does not include any energy penalties associated with sulfur and particulate cleanup in a direct fired system, but includes cleanup in the LBG system.

In general, intercooling of the gasifier product degrades system performance and the magnitude of the degradation increases with turbine inlet temperature. Gasifier intercooling has essentially no effect for the limiting COGAS system in which an atmospheric-pressure furnace-fired exhaust boiler receives hot combustion air from a low temperature gas turbine whose power is a small fraction of the total system power output. On the other hand, there is substantial degradation in a COGAS system where all of the LBG is burned in a high temperature gas turbine combustor and steam is raised only in an unfired waste heat boiler. For high excess air supplementary firing to raise steam either in the gas turbine combustor (supercharged boiler) or the waste heat boiler, intercooling effects are also significant. For the low excess air supercharged boiler there is roughly a 2-1/2 percent degradation in gasifier efficiency due to knocking out the LBG water vapor (roughly 50 percent of the injected steam remains as water vapor in the raw LBG), an effect not present with the atmospheric furnace-fired exhaust boiler. This degradation is not observed if the LBG gas composition is held fixed during intercooling. All of the above conclusions assume utilization of the intercooling heat for feedwater heating and boiling to the extent allowable under the constraints of the particular system.

Supercharged boilers are preferable to fired exhaust boilers and the advantage increases as excess air decreases. Optimum excess air increases with increasing turbine inlet temperature. In making such a comparison it is assumed that the exhaust boiler is fired with an atmospheric gasifier. However, it may be unrealistic to have a separate one-atmosphere gasifier in the high excess air case, and thus advantage of the supercharged boiler may be even more substantial.

At low excess air the supercharged boiler advantage is largely a consequence of gasifier water injection. The additional water vapor in the products of combustion is most effectively utilized by expanding it through the turbine. Thus the advantage of the supercharged boiler becomes considerably more pronounced with LBG than with conventional fuel. Robson(7), for example, shows only a one percentage point advantage for the conventional fuel low excess air supercharged boiler over the fired exhaust boiler. With LBG the advantage can be three percentage points in efficiency.

The supercharged boiler COGAS system with low excess air is less effective than unfired waste heat boiler systems for turbine inlet temperature in excess of 2000°F (low excess air is the optimum firing condition only for inlet temperatures well under 2000°F). However, if the supercharged boiler is optimized with regard to excess air, it then maintains an advantage over other COGAS systems until turbine inlet temperatures are considerably higher, possibly in excess of 2400°F, at which point the unfired waste heat boiler has the advantage.

4.0 ESTIMATES OF NO_x EMISSIONS FROM LBG COMBUSTORS

The analyses in the previous chapter identified the combined gas and steam turbine power plant fired with LBG from an integrated coal gasifier as the most desirable of the advanced power generating systems from a fuel utilization point-of-view. This chapter discusses the NO_x emissions from combustors suitable for this system focusing on NO_x produced by reduction of nitrogen-bearing fuel species such as NH_3 and HCN.

The purpose of this study is to develop an understanding of the important NO_x formation mechanisms and to adjust the combustion parameters of two specific LBG combustors to minimize NO_x. A kinetic model, which includes a reaction set capable of describing NO_x formation and destruction, has been applied to a series of "limit-cases" based on practical operating constraints of combustors fired with ammonia-containing LBG. Although macro-and micro-scale mixing will dictate the NO_x levels in any practical system, this model establishes upper and lower emission limits, and thus, gives an indication of the feasibility of direct use of high ammonia fuel gases.

The next section outlines the methodology for estimating NO_x emissions and describes the kinetic model in more detail. A following section (4.2) describes the fuel and combustor characteristics examined and the last two sections (4.3 and 4.4) give the results for the two specific combustors analyzed.

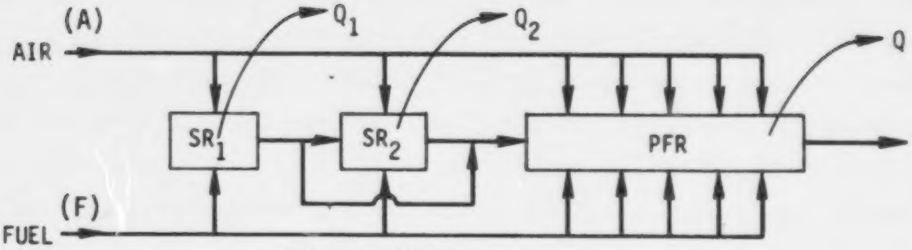
4.1 Methodology for Estimating NO_x Emissions

Having identified two specific combustors of interest, the adiabatic gas turbine and the supercharged boiler, "limit-case" estimates for NO_x emissions were made over a range of system constraints on inlet conditions, fuel composition, and exit conditions.

Limit-case situations are those in which some single aspect of the physics or chemistry dominates and the remaining phenomena can either be ignored or modeled by simple idealized processes. We use the term here to refer to the methodology whereby we search for the lower bounds on NO_x emissions which are set by the chemistry. Implicit in this approach is the assumption that all physical processes associated with fuel-air-product contacting and heat transfer can be accomplished in an ideal and optimum manner dictated by the chemistry. Having established this chemical-lower-bound, the question of how close one can achieve the optimum physical transport behavior is then open to scrutiny.

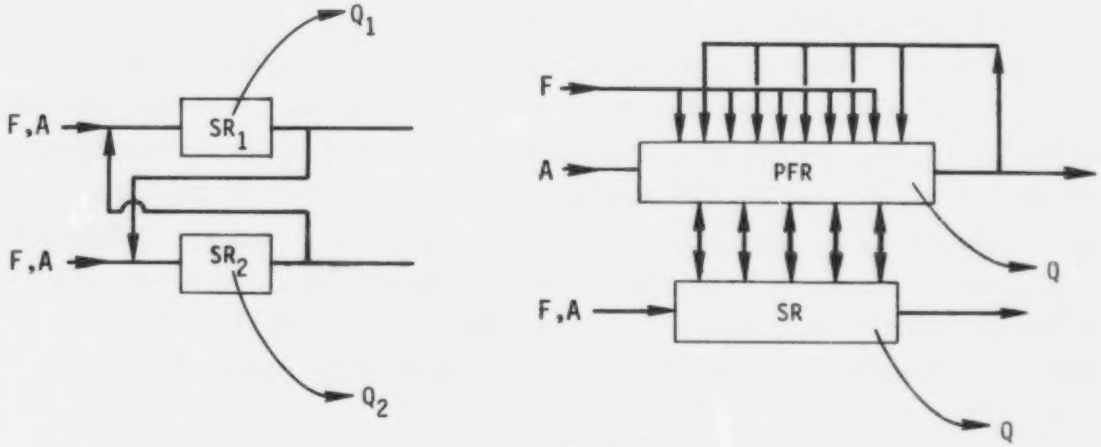
Fundamental to the success of this approach is, of course, an authoritative description of the finite-rate chemistry pertinent to fuel nitrogen (in this instance NH_3) conversion and thermal fixation of N_2. Of particular importance is the inclusion of the proper chemistry to describe the generation of stable intermediate nitrogen compounds (e.g., HCN, NH_3) and their subsequent equilibration path under rich conditions. The role of fuel breakdown and the effect of hydrocarbon radicals on the production and destruction of nitrogen compounds must adequately be described as must the influence of XN compounds on NO_x production and distribution. Appendix C sets forth a proposed kinetic mechanism for NO_x formation in low Btu gas combustion. This set of approximately 100 reactions was employed in all of the NO_x estimates of this investigation. The rationale for selecting this set of reactions and rate constants is described in detail in the appendix.

In searching for the lower bound on NO_x emissions set by the chemistry it is assumed that the optimum chemical reactor system which achieves this lower bound can be described in terms of an interacting set of stirred and plug flow reactors which exchange matter and heat with one another and with the surroundings. The optimum coupling between these basic elements which yields minimum NO_x emissions is unknown at the outset of the search and may indeed be very complex involving several parallel and feedback paths as illustrated in Figure 4-1. The simplest (computationally) of these systems is shown in Figure 4-1a which illustrates a "series" or sequentially-staged set of coupled reactors. SR refers to stirred reactors and PFR to plug flow reactors. Q represents heat loss. The Ultrasystems Modular Kinetics Analysis Program (MKAP) performs the nonequilibrium chemistry and element-to-element bookkeeping on such a coupled system and provides for an arbitrary distribution of mass and energy transfer along the PFR elements. Figure 4-1b illustrates hypothetical systems with feedback loops. In one case the feedback


(A)
AIR
Q_1
Q_2
Q
SR_1
SR_2
PFR
(F)
FUEL

SERIES CONNECTED

4.1a


Q_1
F,A
SR_1
F,A
SR_2
Q_2
F
A
PFR
Q
F,A
SR
Q

FEEDBACK LOOPS

4.1b

Figure 4-1. Examples of Basic Element Coupling for Limit-Case Investigations

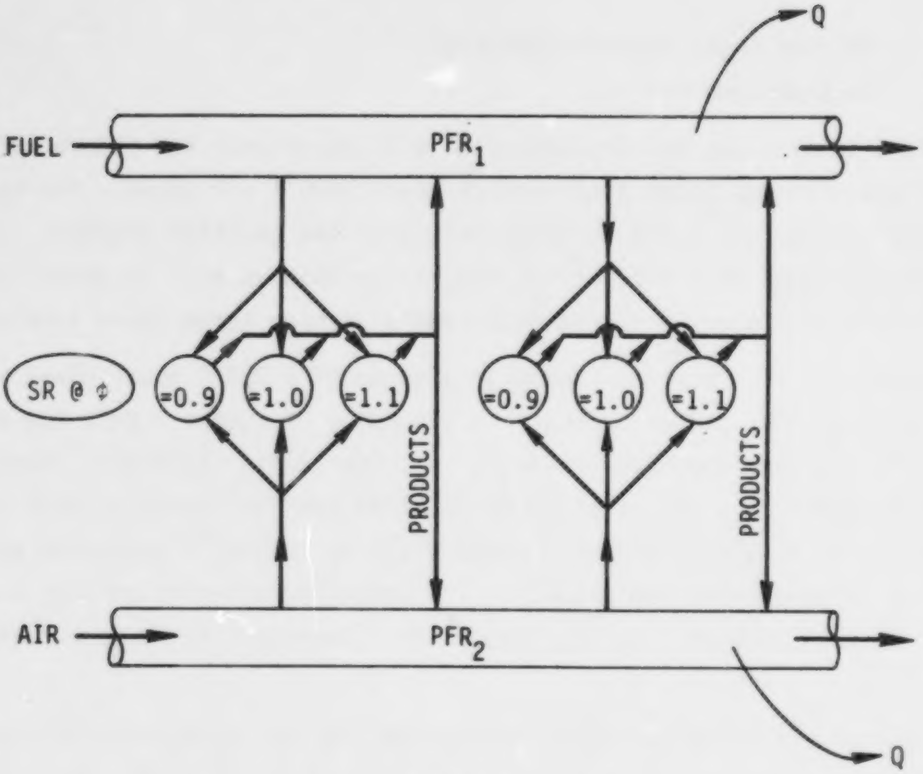
interaction is shown of two well-stirred zones with different residence times and heat loss factors. The other illustration shows a plug flow zone with distributed feedback from both exhaust products and from a well-stirred zone. Such a system might be used for example, to model a free shear layer combustion zone with distributed fuel addition which is stabilized through coupling to a recirculation zone, and which is further complicated by the presence of external exhaust gas recirculation. Figure 4-1c shows examples of "parallel" couplings in which no influence of downstream behavior is felt upstream. However, continuous exchange between reactor elements is allowed. The upper sketch indicates how parallel couplings of this sort can be used to simulate diffusion flame behavior wherein the flame zone is modeled by a distribution of stirred reactors at various equivalence ratios. The products from this flame zone are then transported back to the lean and rich sides of the flame.

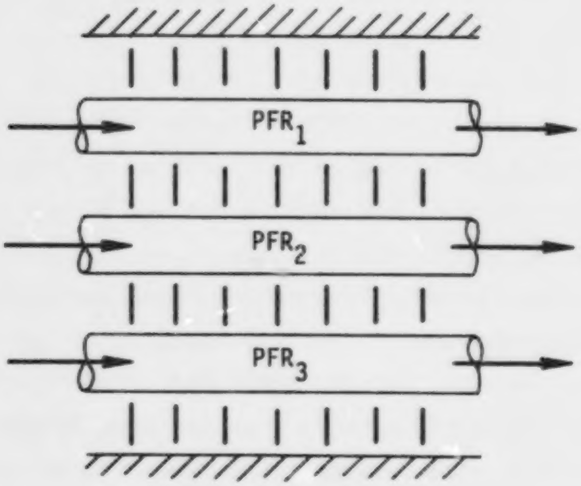
A definitive methodology for determining the optimum interacting set of reactors is not known at present, and is the subject of current theoretical and experimental research. For the purposes of this study, we have adopted a simpler notion. It has been assumed that a close estimate for the lower NO_x emission bound set by the chemistry can be obtained by examining a simple series coupling of a rich primary plug flow reactor followed by a secondary reactor which completes the combustion and achieves the correct combustor exit conditions. The combined system of reactors is subject to certain design constraint bounds on overall heat transfer rates and residence times (size).

The principle variables over which an optimum was sought are primary zone equivalence ratio, temperature, and residence times and secondary zone combustion air entrainment rate and heat transfer rate. The SR and PRF subelements of the MKAP program are standard chemical kinetic calculation routines using fully implicit integration. They are documented in Reference 18.

4.2 General Characteristics of Combustors and Selected Fuel

The analyses in Section 3 point to two types of combustors for use in advanced power generating systems designed for optimum fuel utilization. The following combustors were selected for the NO_x emission studies.


Q
FUEL
PFR1
SR @ ϕ
=0.9
=1.0
=1.1
=0.9
=1.0
=1.1
PRODUCTS
PRODUCTS
AIR
PFR2
Q


PFR1
PFR2
PFR3

4.1c
Parallel Connected Elements

Figure 4-1. Examples of Basic Element Coupling for Limit-Case Investigations (Continued)

- Adiabatic gas turbine combustor
- Supercharged boiler

The adiatatic gas turbine combustor will be optimum for future COGAS systems when turbine inlet temperatures reach 2400^{0}F and above. For maximum performance it will require no intercooling of the gasifier product. It is implicitly assumed that hot gas H_2S removal techniques will be developed on a time scale consistent with the development of high temperature turbines.

Figure 4-2 is a partial schematic diagram of a COGAS power plant with integrated gasifier and an adiabatic gas turbine combustor. Only the major heat, work and mass flows important to combustor design have been shown. The compressor feeds both the pressurized gasifier and the combustor with compressed air at 10 atmospheres and temperature up to 1000^{0}F depending upon the degree of recouperation (not shown). The combustor operates at high excess air to maintain combustor outlet temperature (turbine inlet temperature) at 2800^{0}F.

A low excess air supercharged boiler firing low temperature LBG from an intercooled gasifier with a turbine inlet temperature of 2000^{0}F was selected as the second combustor for this study for three reasons. First, as distinct from the adiabatic high temperature gas turbine combustor, this combustor represents the optimum choice for a COGAS system when restricted to present state-of-the-art technology in regard to H_2S clean up and turbine inlet temperature limitations. Second, although the choice of low excess air is not necessarily optimum for 2000^{0}F turbine inlet temperature it is representative of designs suitable for use with low turbine inlet temperatures and it serves as a vehicle to illustrate the distinctive features of low excess air firing as distinct from the pure gas turbine combustor. And third, the supercharged boiler appears to be the optimum choice for the near future operating at higher excess air levels with turbine inlet temperatures approaching 2400^{0}F. Hence, its study at this time is pertinent not only to immediate COGAS system development, but also to developments over the next decade.

Figure 4-3 is a partial schematic diagram of a COGAS power plant with a supercharged boiler. A heat exchanger and low temperature cleanup system have replaced the high temperature cleanup system in the previous example

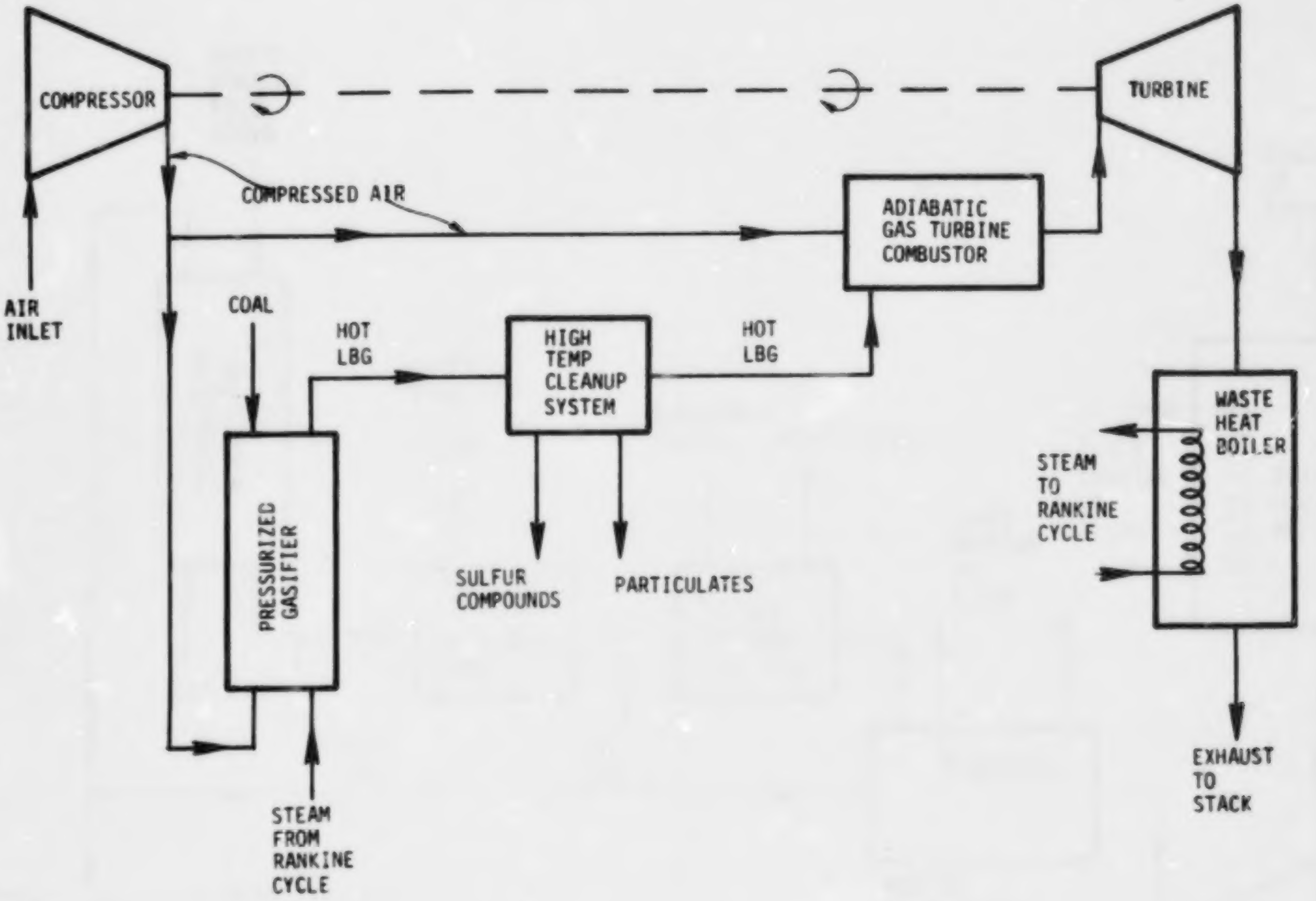

COMPRESSOR
TURBINE
AIR INLET
COMPRESSED AIR
ADIABATIC GAS TURBINE COMBUSTOR
COAL
HOT LBG
HIGH TEMP CLEANUP SYSTEM
HOT LBG
PRESSURIZED GASIFIER
SULFUR COMPOUNDS
PARTICULATES
STEAM FROM RANKINE CYCLE
WASTE HEAT BOILER
STEAM TO RANKINE CYCLE
EXHAUST TO STACK

Figure 4-2. COGAS Power Plant with Adiabatic Gas Turbine Combustor

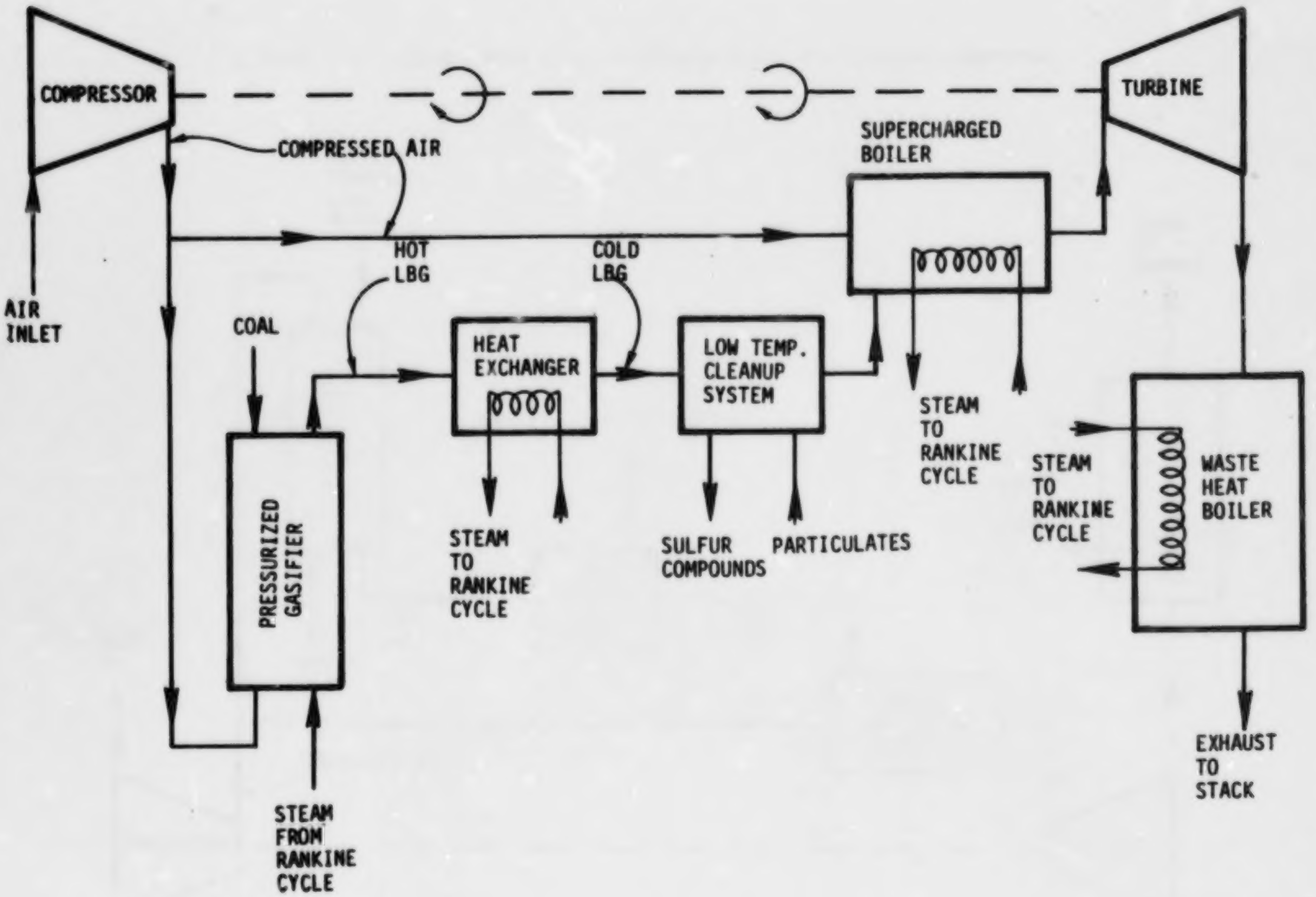

COMPRESSOR
TURBINE
COMPRESSED AIR
AIR INLET
HOT LBG
COLD LBG
SUPERCHARGED BOILER
COAL
HEAT EXCHANGER
LOW TEMP. CLEANUP SYSTEM
PRESSURIZED GASIFIER
STEAM TO RANKINE CYCLE
STEAM TO RANKINE CYCLE
STEAM TO RANKINE CYCLE
WASTE HEAT BOILER
SULFUR COMPOUNDS
PARTICULATES
EXHAUST TO STACK
STEAM FROM RANKINE CYCLE

Figure 4-3. COGAS Power Plant with Supercharged Boiler

and the LBG is assumed to enter the combustor at 150°F. The supercharged boiler operates with low excess air (nominally 5 percent) and outlet temperature is controlled by heat removal to the Rankine cycle.

Table 4-1 summarizes the characteristics of the two combustors selected for analysis.

Table 4-1. Combustor Parameters

Parameter	Adiabatic Gas Turbine Combustor	Supercharged Boiler Combustor	Units
Air temperature	1000	600	°F
Air pressure	10	10	atm
Fuel gas temperature	1500	150	°F
Fuel gas pressure	10	10	atm
Outlet temperature	2800	2800	°F
Excess air	High	5	%
Heat removal	No	Yes	—

Unfortunately, the selection of a fuel gas for analysis is not as straightforward. Section 2 demonstrated that the properties of LBG vary considerably depending upon gasifier design and operation and the characteristics of the coal feed and other inputs. Since the purpose of this analysis is to examine the formation of NO_x, and in particular, the contribution of nitrogen-bearing fuel species and the role of hydrocarbons, the fuel described in Table 4-2 was selected. This LBG has a species distribution similar to that produced by an air-blown (LBG) gasifier as listed in Table 2-1. Since the LBG is assumed to enter the combustor after a cleanup process, the H_2S and COS components were eliminated. The fuel was then doped with 4000 ppm of ammonia, an amount estimated by Robson(7), as a potential level associated with high temperature gas cleanup.

Table 4-2. LBG Composition Assumed for NO_x Study

Specie	Mole %
H_2O	10.1
H_2	19.6
CO	13.3
CO_2	13.3
CH_4	5.5
N_2	37.6
NH_3	Up to 0.4

4.3 Adiabatic Gas Turbine Generator Results

In order to establish the chemical constraints on the control of NO_x formation in adiabatic gas turbine combustors burning LBG, a set of numerical computations was performed using the MKAP methodology outlined in Section 4.1. The intent of these computations was to expose the dominant chemical mechanisms leading to NO_x formation and destruction and to establish their dependence on the gross design features of gas turbine combustors. An additional goal was to set estimates on the lower achievable limits of NO_x emissions as dictated by chemical considerations.

4.3.1 General Flame Characteristics

The first group of calculations was done to establish general combustion characteristics of the selected LBG fuel gas such as flame temperature variation with stoichiometry and autoignition temperature for premixed fuel and air at the inlet conditions. The peak adiabatic flame temperature is 3660°F and occurs at an equivalence ratio of 1.05. This high value* is due to the compensating effects of:

- high air preheat (due to air compression in both the gasification and final combustion processes)

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*Approximately 75°F less than adiabatic flame temperature for coal/air with room temperature air and 100°F higher than that for methane/air.

- losses associated with the Lurgi process due to water addition (dilution and latent heat effect), heat loss and tar losses.

An overall equivalence ratio of 0.45 corresponds to the desired turbine inlet temperature of 2800^{0}F.

Using the MKAP program it was found that the autoignition temperature for this fuel is approximately 1400^{0}F over a broad range of fuel/air ratio. This is on the order of 100^{0}F above the unignited mixture temperatures for all but very rich mixtures, and hence, for the premixed conditions of interest here an external energy source or backmixing of hot products is required for ignition and flame stability. For the numerical experiments performed in this study a 1.0 msec residence time adiabatic-stirred reactor was used to provide ignition. In the limit of very rapid initial mixing this is a reasonable representation of the ignition process, although residence times may be considerably longer. Slower mixing of the reactant (even in the absence of backmixing) may give rise to diffusion zones which can attain autoignition conditions in locally-rich regions without the presence of an ignition source.

The effect of ignition zone residence time is examined later in the study. In general, it is found that if the stirred reactor residence time is increased while maintaining total (plug flow and stirred reactor) residence time fixed, then there is little effect for fuel-lean systems. Under rich conditions, systems with larger stirred reactors appear to be richer in their general characteristics with higher concentrations of hydrocarbon fragment and lower concentrations of oxidative radicals.

4.3.2 Premixed Lean Combustion

Having determined these flame characteristics, the second task was to establish the NO_x emission levels under premixed conditions at the overall equivalence ratio of 0.45. This situation then becomes a point of departure to examine other staged combustor concepts. It serves as a useful yardstick with which to measure NO_x control effectiveness. Figure 4-4 shows a schematic of the simple MKAP analogy to this situation where a stirred reactor ignition region is followed by an adiabatic plug flow reactor. Figure 4-5 shows the NO growth with time at pressures of 1 and 10 atmospheres for the case of zero

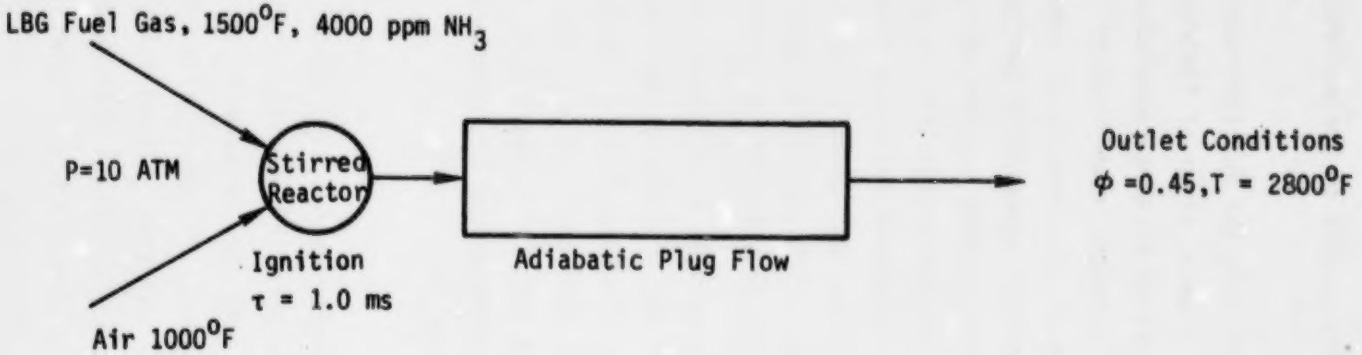
LBG Fuel Gas, 1500°F, 4000 ppm NH_3
P=10 ATM
Stirred Reactor
Air 1000°F
Ignition
τ = 1.0 ms
Adiabatic Plug Flow
Outlet Conditions
φ =0.45,T = 2800°F

Figure 4-4. Premixed Adiabatic Gas Turbine Combustor — MKAP Analog Schematic

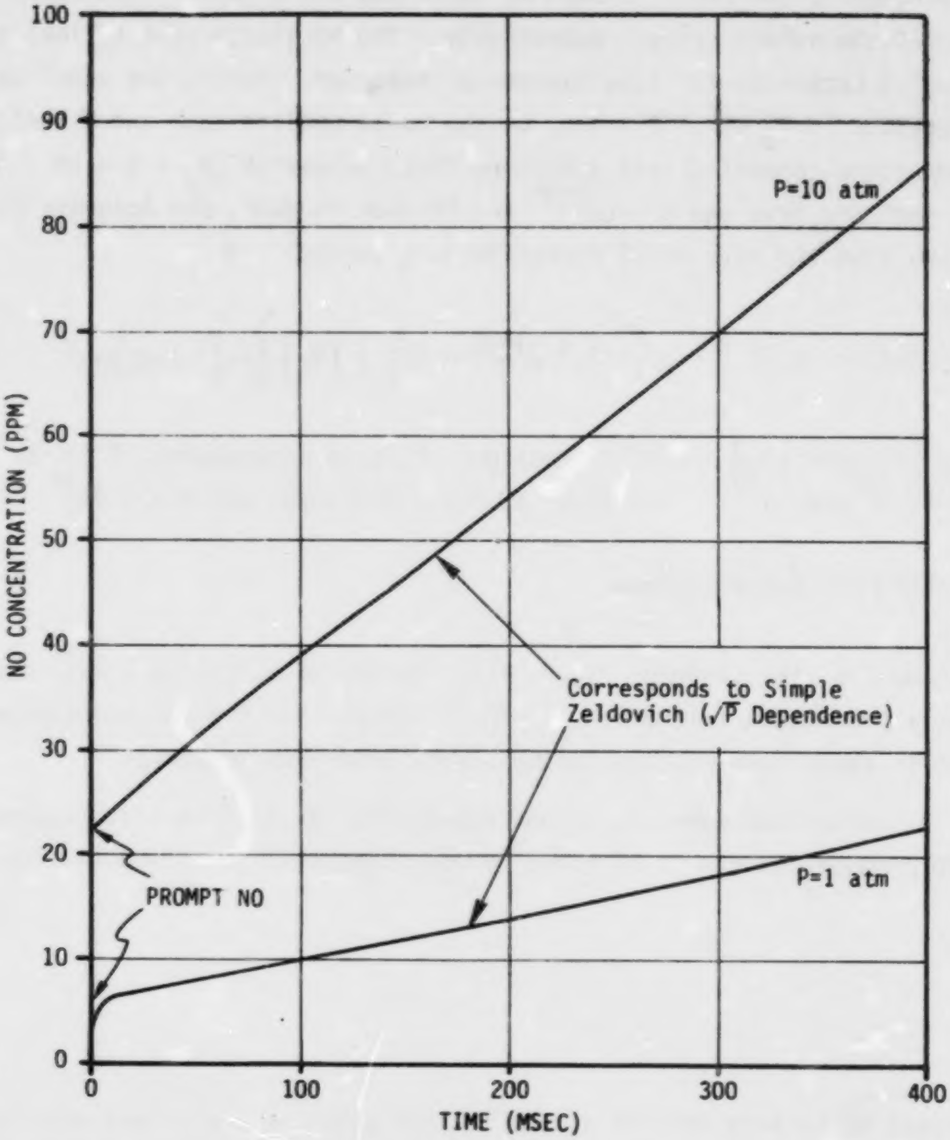

Figure 4-5. NO from Lean Premixed Combustion — Adiabatic Gas Turbine Combustor — No Fuel Ammonia

NOTE: $\phi = 0.45$; $T_{outlet} = 2800^{o}F$; $(NH_3)_0 = 0.0$

NH_3 content in the fuel. Prompt NO[*] of 6 ppm and 23 ppm is indicated for the 1 and 10 atmosphere cases, respectively. The NO growth rate follows the simple Zeldovich mechanism for lean systems as expected. Making the usual Zeldovich assumptions (O/O_2 equilibration, NO far below equilibrium, and N radicals at steady state concentration) and using first Zeldovich ($N_2 + O \rightarrow NO + N$) reaction rate constant from the Baulch(19) (as is used in MKAP, see Appendix C) then it follows that the rate of NO formation is given by

$$[N\dot{O}] = 0.21 \left| \exp\left[-37.4 \left(\frac{1800}{T} - 1\right)\right] \right| \left[N_2\right] \left[O_2\right]^{\frac{1}{2}} \left(\frac{P}{T/1800}\right)^{\frac{1}{2}}$$

where $\left[N_2\right]$ and $\left[O_2\right]$ are mole fractions, P is in atmospheres, T is in ^{o}K, and $[N\dot{O}]$ is in ppm/msec. This gives at P =1, T = 1800, and $\phi = 0.45$[**]:

$$[N\dot{O}] = 0.044 \text{ ppm/msec}$$

which matches the slope of Figure 4-5. Furthermore, the 10 atmosphere curve shows a production rate which is $(10)^{\frac{1}{2}}$ higher than the one atmosphere slope which is again consistent with the simple Zeldovich mechanism.

A similar and more convenient expression for the temperature dependence of NO production rate is obtained by logrithmetically differentiating the

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[*] Prompt NO is here defined as the extrapolation of the linear portion of the curves to zero time. It includes the NO produced in the 1.0 msec stirred reactor which is primarily a consequence of high superequilibrium O-atm concentrations.

[**] For the assumed LBG composition the N_2 and excess O_2 mole fractions are (with CO_2 and H_2O products of combustion):

ϕ	$T_f(^{o}F)$	N_2	O_2
.45	2800	.68	.085
.53	3000	.67	.069

above Zeldovich expression and approximating the resulting expression for temperatures near 3000^{0}F. Thus:

$$\frac{d[\dot{\mathrm{NO}}]}{[\dot{\mathrm{NO}}]} = d\left[-37.4\left(\frac{1800}{T} - 1\right)\right] - \frac{1}{2}\,\frac{dT}{T}$$

$$= \left[\frac{37.4(1800)}{T} - \frac{1}{2}\right]\frac{dT}{T}$$

which for T $\doteq$ 3000^{0}F (1922^{0}K) gives

$$\frac{d[\dot{\mathrm{NO}}]}{\dot{\mathrm{NO}}} \doteq 35\,\frac{dT}{T}$$

or

$$[\dot{\mathrm{NO}}] \propto T^{35}.$$

A 100^{0}F increase in temperature roughly triples the NO production rate.

Figure 4-6 presents the same calculation as shown in Figure 4-5 except that the flame temperature has been increased to 3000^{0}F (ϕ=0.53). The NO production rate at 3000^{0}F is approximately six times that at 2800^{0}F which reflects the temperature increase as well as the slight reduction in N_2 and excess O_2 concentrations*. On the other hand, note that the prompt NO (including that formed in the 1.0 msec stirred reactor) has increased only by a factor of two which implies that O-O_2 equilibration is more rapid at higher temperatures with an attendant lower fractional overshoot.

In an attempt to rationalize the prompt NO level in Figure 4-5 the oxygen atom superequilibrium overshoot has been plotted in Figure 4-7. The very high levels in the 1.0 msec stirred reactor and during the first two milliseconds of the plug flow reactor are responsible for the prompt NO production.

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*This is somewhat less of an increase than predicted by the simple Zeldovich mechanism.

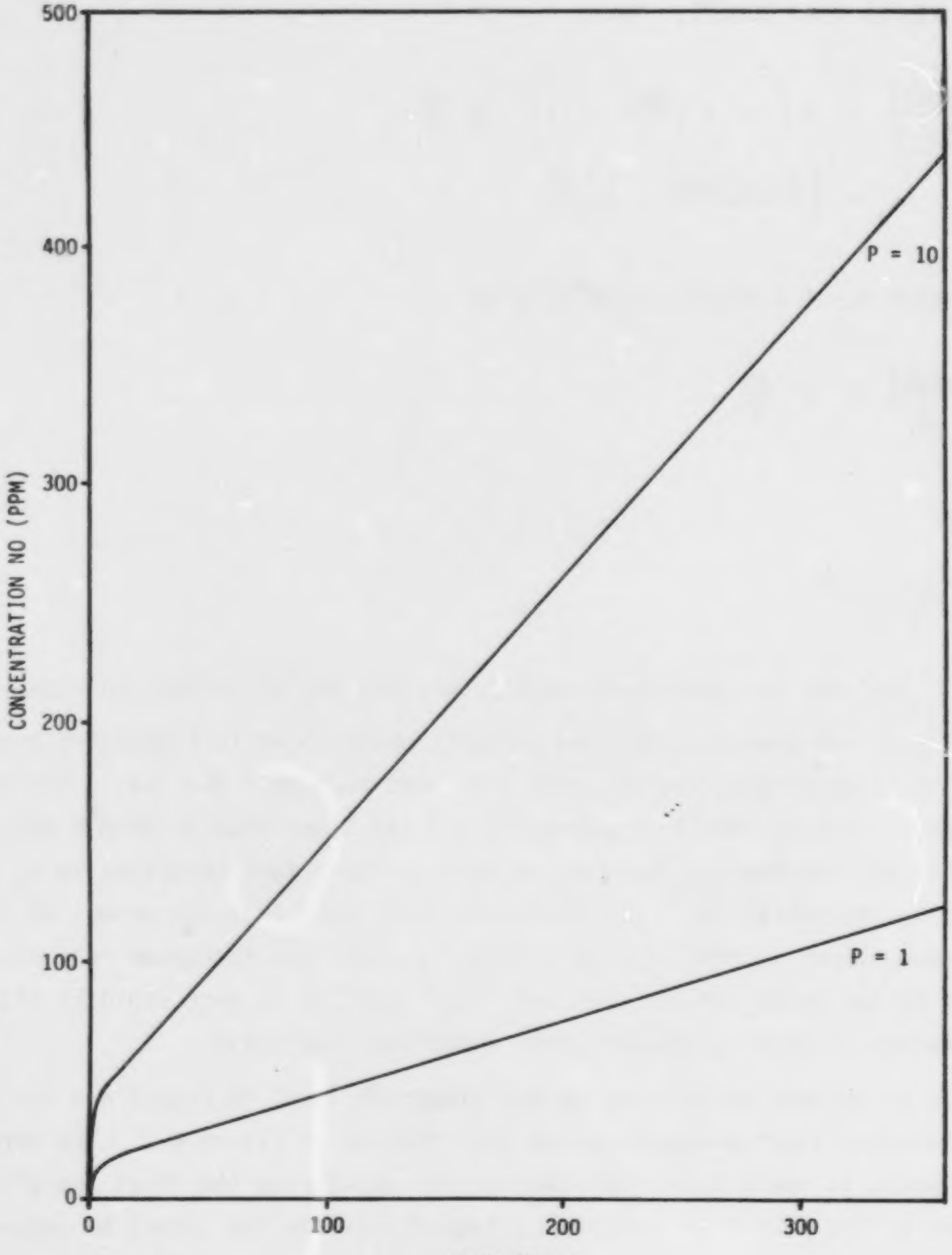


Figure 4-6. NO from Lean Premixed Combustion — Adiabatic Gas Turbine Combustor — No Fuel Ammonia

NOTE: $\phi = 0.53$; $T_{outlet} = 3000^{o}F$: $(NH_3)_0 = 0.0$

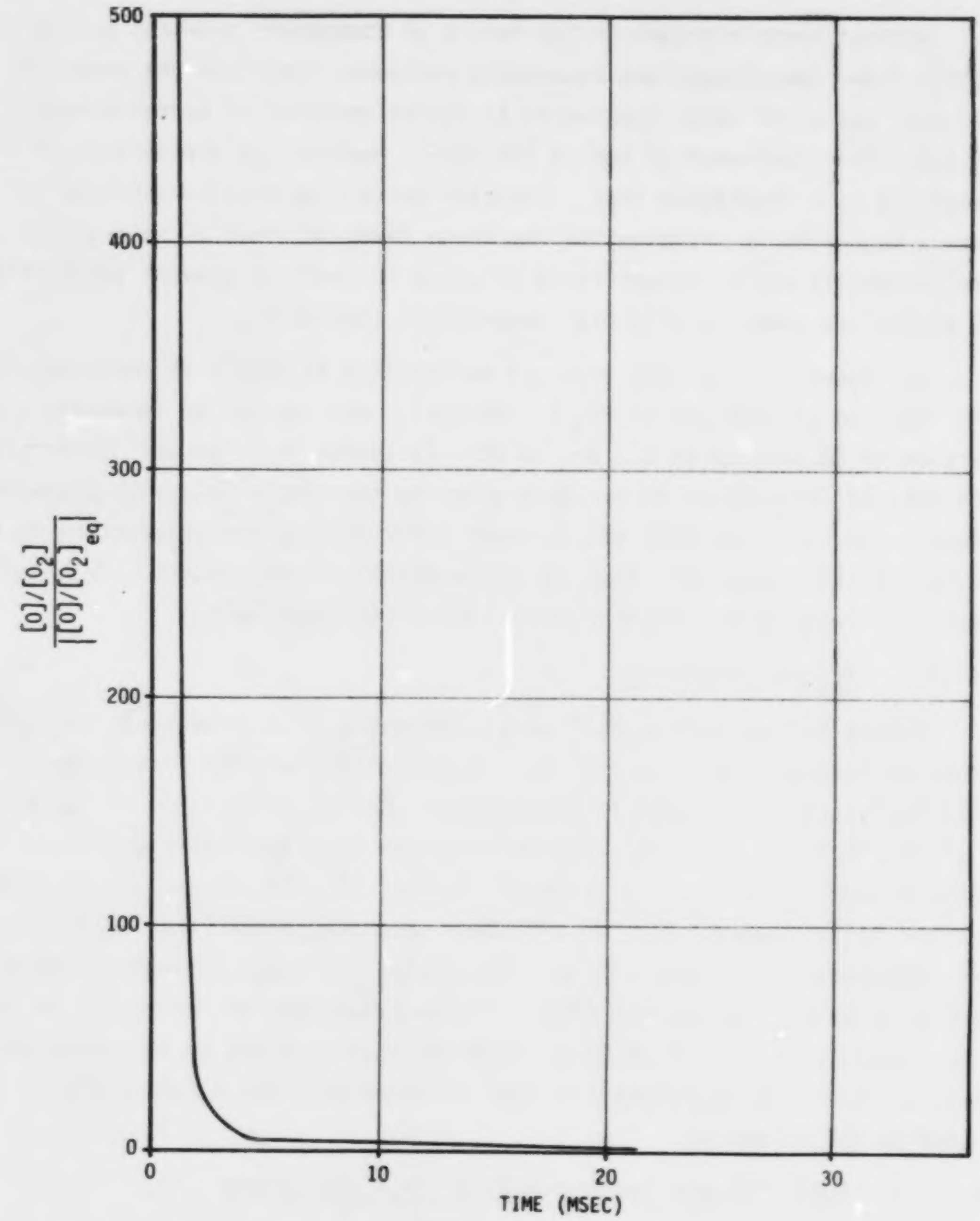


Figure 4-7. Superequilibrium O Concentration, Lean Premixed Combustion — Adiabatic Gas Turbine Combustor

NOTE: $\phi = 0.45$; $T_{outlet} = 2800°F$; $P = 1.0$ atm; $(NH_3)_0 = 0.0$

Without bound nitrogen in the fuel a 10 atmosphere premixed system at $2800^{\circ}F$ flame temperature and reasonable residence times (on the order of 100 ms), has an NO level (corrected to stoichiometric) of approximately 85 ppm. The attainment of such a low level, however, in the absence of premixing is a formidable task. Fuel/air contacting must be achieved in such a manner as to minimize the residence times in zones of near-unity stoichiometric ratio through rapid dilution in order to prevent substantial NO production under locally high temperature conditions.

In Figure 4-8 the same premixed calculation at $2800^{\circ}F$ is repeated with the addition of 4000 ppm of NH_3 in the fuel. Here we see an immediate conversion of 86 percent of the NH_3 to NO. Following this "prompt" conversion the rate of increase of NO is again given by the simple Zeldovich mechanism. Clearly the resulting 2000 ppm NO level (corrected to stoichiometric) is an indication that more effective control measures must be sought. The next series of calculations examine other control alternatives.

4.3.3 Staged Combustion

Figure 4-9 presents a MKAP analog schematic of a large-scale gas turbine combustor concept based on staging. A long residence time rich primary "hold-up" zone is provided in anticipation that it is possible to "cook" the fuel NH_3 to N_2 in an oxygen-depleted environment given sufficient time. The primary zone is followed by secondary burnout and dilution to the desired turbine inlet temperature. In this lean secondary process any residual nitrogen compounds will convert to NO. The design challenge for the secondary and dilution zones is to avoid diffusion flame production of thermal NO in locally hot, near-stoichiometric regions. One possibility would be to reduce the primary zone exit temperature by heat exchange with the dilution air as indicated in the schematic.

4.3.3.1 Fuel Nitrogen Conversion Under Rich Conditions

The nonequilibrium chemistry associated with the transfer of fuel nitrogen to N_2, NO, or HCN in a rich primary is complex and not well-understood. However, two significant results can be derived from an examination of the

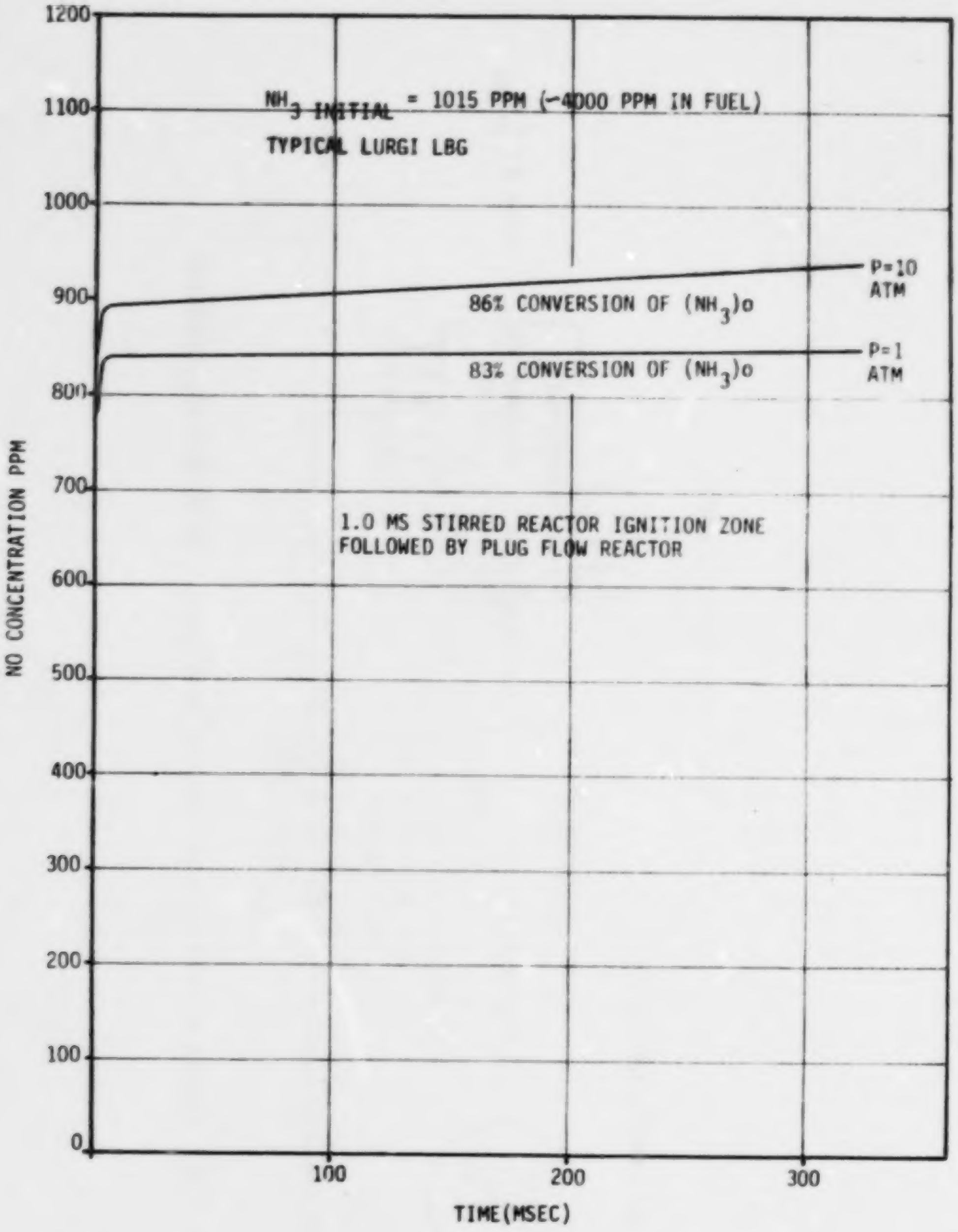


Figure 4-8. NO from Lean Premixed Combustion — Adiabatic Gas Turbine Combustor — With Fuel Ammonia

NOTE: $\phi = 0.45$; $T_{flame} = 2800^{o}F$

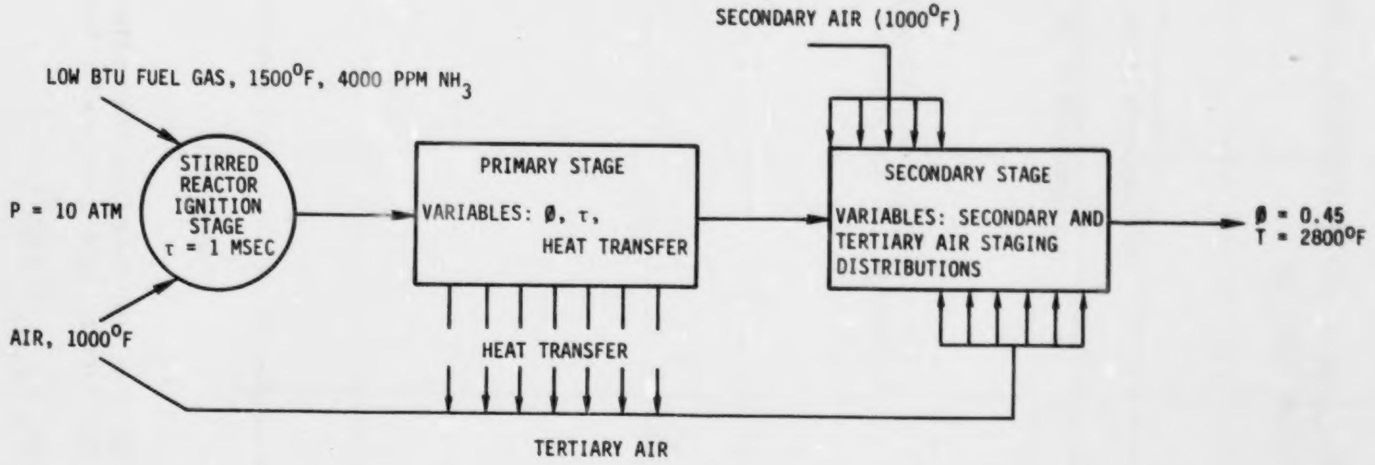

LOW BTU FUEL GAS, 1500°F, 4000 PPM NH_3
P = 10 ATM
STIRRED REACTOR IGNITION STAGE
τ = 1 MSEC
AIR, 1000°F
PRIMARY STAGE
VARIABLES: Ø, τ, HEAT TRANSFER
HEAT TRANSFER
TERTIARY AIR
SECONDARY AIR (1000°F)
SECONDARY STAGE
VARIABLES: SECONDARY AND TERTIARY AIR STAGING DISTRIBUTIONS
Ø = 0.45
T = 2800°F

Figure 4-9. Staged Adiabatic Gas Turbine Combustor — MKAP Analog Schematic

numerical results presented in this section. First, in the moderately rich primary combustion process a "prompt" transfer of fuel N to N_2 occurs within the first millisecond which can account for two-thirds of the effectiveness of the primary zone. This prompt reduction of fuel N is accompanied by a significant generation of superequilibrium HCN and NO. Ideally then the function of the subsequent long primary hold-up period is to drive all of the remaining N-containing constituents to their low equilibrium values. Under very rich conditions this goal is thwarted by further synthesis of superequilibrium HCN followed by a freezing-out due to the slow HCN destruction process under rich conditions.

The second result is associated with the long primary hold-up zone. After a period of 100-200 msec the composition becomes independent of the initial level of NH_3 for a broad range of primary zone stoichiometry (ϕ = 0.8 - 1.7). On the lean side this is merely a statement that equilibrium has been reached. At intermediate equivalence ratios ($\phi \doteq 1.3$) it is indicative of reaching a universal approach-to-equilibrium condition. Under richer conditions (ϕ=1.67) it represents the achievement of a common approach-to-equilibrium for NO and NH_3. Further, under these rich conditions (ϕ=1.67) the HCN nonequilibrium synthesis and freezing processes are dominated by Fenimore-type reactions, and hence, are independent of the initial NH_3 levels.

Before proceeding with a presentation of the primary zone numerical calculations it is appropriate to suggest possible chemical mechanisms which dominate the early NO formation period. Figures 4-10 and 4-11 present nitrogen balance diagrams from 2-msec residence time stirred reactor calculations for methane-air combustion at an equivalence ratio of 1.33. They are pertinent to this discussion because they are doped in one case with a high initial NO level (1300 ppm) and in the other with a high initial NH_3 level (1300 ppm), and the overall results of these calculations compare well with stirred reactor data obtained at Exxon (see Appendix C). The circles represent the various significant nitrogen species which exchange N with one another via the reaction paths indicated by connecting lines. The molecular partner in the forward direction is indicated on the line and the direction is signified by the arrowhead. The numbers within the circles represent the net production rate of the N-containing molecule. All rates have the units of ppm per msec. Finally,

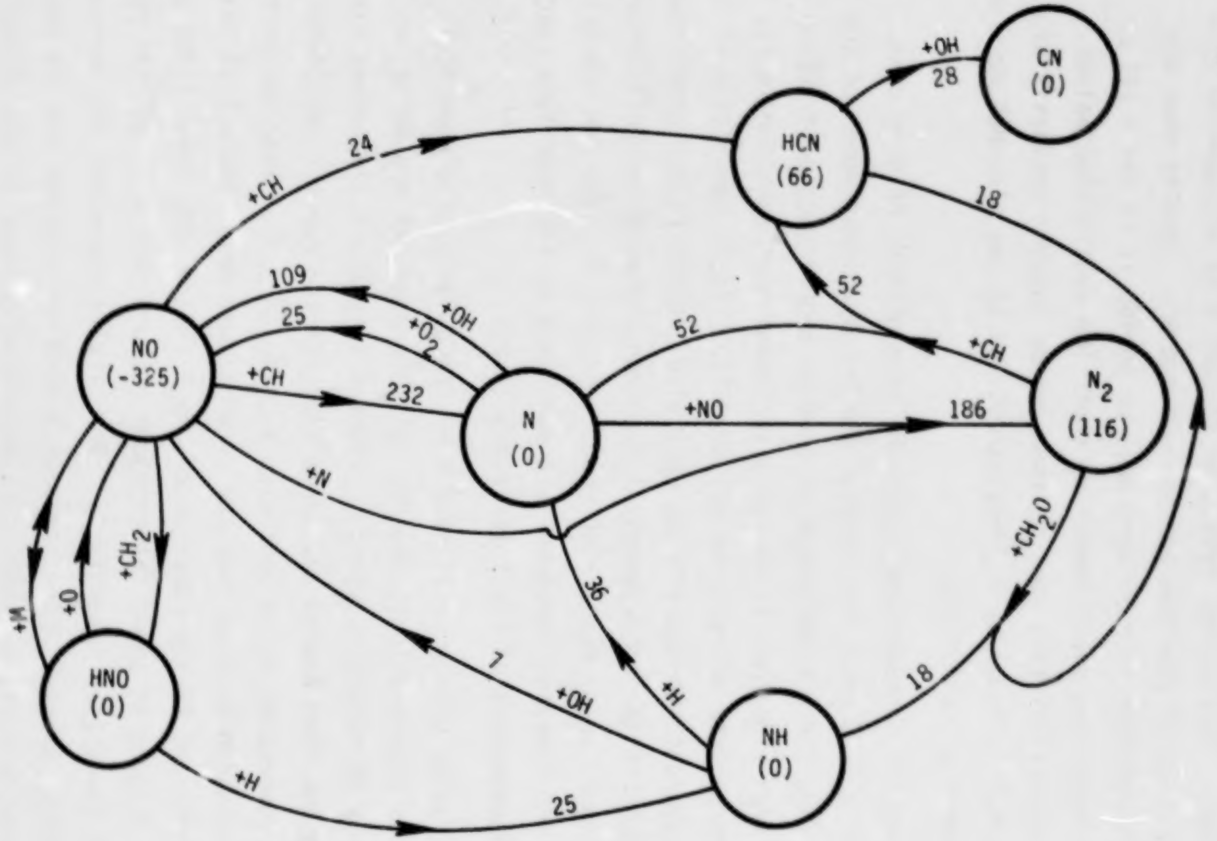

CN
(0)
+OH
28
HCN
(66)
24
+CH
18
52
109
+OH
25
+O2
52
+CH
NO
(-325)
+CH
232
N
(0)
+NO
186
N2
(116)
+N
+CH2O
36
+CH2
+O
+M
7
+OH
+H
18
HNO
(0)
NH
(0)
+H
25

Figure 4-10. NO Formation and Destruction in Well-Stirred CH_4 — Air Reactor with 1300 ppm NO Addition

NOTE: Equivalence Ratio = 1.33; Residence Time = 2 msec

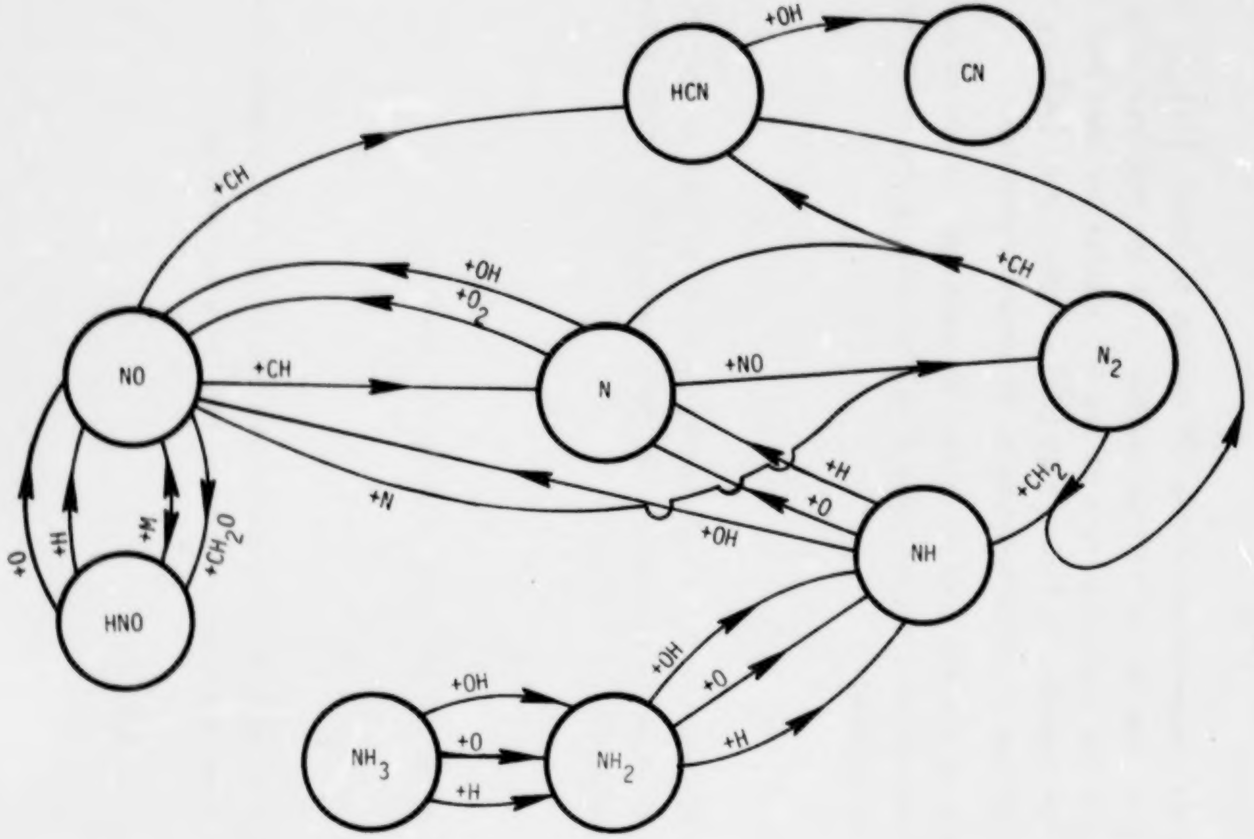

HCN
CN
+OH
+CH
+OH
$+O_2$
+CH
NO
+CH
N
+NO
N_2
+H
+O
+OH
+N
$+CH_2$
NH
+O
+H
+M
$+CH_2O$
HNO
+OH
+O
+H
NH_3
NH_2
+OH
+O
+H

Figure 4-11. NO Formation and Destruction in Well-Stirred Reactor with 1300 ppm NH_3 Addition

NOTE: Equivalence Ratio = 1.33; Residence Time = 2 msec the concentrations of the various nitrogen molecules are given by a mass balance across the reactor.

$$\left[C_i\right] - \left[C_i\right]_{init} = \tau\left[\dot{C}_i\right]$$

where $\left[C_i\right]$ is the concentration of the i^{th} species in (ppm), $\left[C_i\right]_{init}$ is the concentration entering the stirred reactor, τ is the residence time in msec, and $\left[\dot{C}_i\right]$ is the production rate of the i^{th} species per unit mass in the reactor. For example, in Figure 4-10 $[\dot{NO}] = -325$, $\tau = 2$, $[NO]_{init} = 1300$. Hence, $[NO] = 650$ ppm which corresponds to 50 percent retention.

Figure 4-10 is for the case of initial NO addition. It can be seen that N atom production and destruction plays a central role in the prompt decay of NO. The Myerson reaction

$$NO + CH \rightarrow CHO + N \qquad (1)$$

appears to be responsible for direct reduction of NO as well as producing N atoms. These NO atoms in turn enter into both: production of NO, primarily via the extended Zeldovich reaction

$$N + OH \rightarrow NO + H, \qquad (2)$$

and reduction of NO via the reverse Zeldovich reaction

$$NO + N \rightarrow N_2 + O \qquad (3)$$

The destruction of NO by N outweighs production of NO by N roughly in the ratio 4:3. N atoms are also produced by the Fenimore reaction

$$CH + N_2 \rightarrow HCN + N \qquad (4)$$

Although this promotes reduction of NO it is also the primary producer of HCN. How effectively HCN is subsequently removed in the hold-up zone (if at all) is unclear. The other Fenimore reaction

$$CH_2 + N_2 \rightarrow HCN + NH \tag{5}$$

is substantially less effective in this instance as a producer of HCN. The NH so produced has little overall effect on NO production or destruction as can be seen from the balance diagram. Sufficient N atoms are formed from

$$NH + H \rightarrow N + H_2 \tag{6}$$

to provide an NO sink which compensates for the small NO production through

$$NH + OH \rightarrow NO + H_2 \tag{7}$$

Approximately 25 percent of the HCN production is through a direct conversion of NO via the Myerson reaction

$$NO + CH \rightarrow HCN + O. \tag{8}$$

This, however, accounts for less than 10 percent of the NO destruction. Finally, an active loop exists between NO and HNO. Although this loop has only a small (less than 10 percent) direct effect on NO depletion, it does effect the O, OH and H radical population, and hence, exerts an indirect effect.

With this background on prompt behavior with large initial NO levels we now examine Figure 4-11 which is more representative of the situation at hand. In this instance the stirred reactor is doped with 1300 ppm of ammonia. The process is essentially a cascading down from NH_3 to N as shown. This large N atom source in the absence of high initial NO concentrations provides a net source of NO primarily from the extended Zeldovich reaction (2). The production of NO by N outweighs the destruction of NO by N in the ratio 1.6:1. NO is depleted by the Myerson reaction (1) and the reverse Zeldovich reaction (3) which leads to N_2 and is the final link in the transfer of nitrogen from

NH_3 to N_2. The Fenimore reactions (4) and (5) act to provide a net production of NO through the generation of N atoms. These reactions are again a source of HCN. With the reaction scheme used in this study the linkage between NH_3 and HCN is through NO generation from NH_3 followed by the Myerson reaction (8). In the case at hand this linkage is weak with only a small portion of the HCN so generated. It is possible, however, that under different equivalence ratios the NH_3-HCN linkage could be stronger. The NO-HNO loop again appears primarily as a factor in the O, OH, and H radical balance. The small time constant of the initial or "prompt" NH_3 conversion is clearly associated with the rapid methane combustion process producing hydrocarbon fragments as intermediaries and with the rapid decomposition of NH_3 yielding N atoms under rich conditions.

The effect of residence time and degree of backmixing on "prompt" behavior has not been thoroughly explored. In general it was found that under relatively lean conditions there is no discernable difference between a longer residence time stirred reactor and a stirred reactor followed by a plug flow section with the same total residence time. However, under richer conditions ($\phi \geq 1.2$) it was found that the longer residence time stirred reactors behaved as if they were operating under richer conditions when compared to short residence time stirred reactors followed by a plug flow section.

4.3.3.2 Fuel Rich Primary Stage - Baseline Case

This section presents the results of detailed kinetic calculations applied to a baseline fuel-rich primary stage. The basic combustion arrangement is shown in Figure 4-9 and incorporates the following features:

- LBG fuel gas (composition listed in Table 4-2)
- Pressure 10 atm
- Oxidant is air at 1000°F
- Fuel temperature is 1500°F
- Stirred reactor residence time is 1 ms

The following discussion addresses the NO_x kinetics for the baseline reactor as the following parameters are varied:

- Equivalence ratio, ϕ
- Adiabatic plug flow residence time, τ

- Initial fuel ammonia content, $(NH_3)_0$
- Air nitrogen replacement by Argon

The discussion is necessarily speculative due to considerable uncertainties in the basic chemical kinetic set and rate constants employed in the calculations.

Equivalence Ratio and Plug Flow Residence Time

Figures 4-12 to 4-15 show the nitrogen species history for an adiabatic plug flow rich primary at various equivalence ratios (2.0, 1.67, 1.33, 1.1). Essentially all of the "prompt" behavior has been completed within the stirred reactor ignitor and the subsequent behavior is slowly varying as seen in these figures. The stirred reactor output is plotted along the ordinate. The solid curves are for the fuel NH_3 concentration set equal to zero. Figure 4-16 is a similar calculation under lean conditions (ϕ=0.9) included here for comparison.

In examining the primary zone behavior for various equivalence ratios there are several aspects to scrutinize. First, how effective was the prompt reduction of nitrogen compounds (that is, NO precursors which will convert to NO in the secondary stage)? What is the distribution of these species? How effective is the rich hold-up zone in promoting equilibration of these species? To what degree does nonequilibrium generation of HCN take place? Under what conditions does the HCN level freeze? Does the system reach a condition which is independent of the initial fuel nitrogen level?

Figure 4-12 presents the results for the richest case (ϕ=2.0) examined. More than 80 percent of the fuel N is still present as NO precursors following the stirred reactor. The system is too rich and most of the NH_3 does not decompose in the stirred reactor. The NH_3 which does decompose, converts primarily to N_2 with approximately 150 ppm of NO also appearing. With time the NH_3 and NO slowly decay towards their equilibrium values. Although very little HCN appears initially, nonequilibrium synthesis of HCN proceeds throughout the entire period apparently due to nonequilibrium hydrocarbon fragments participating in the Fenimore-type reactions. The indirect conversion of NH_3 to HCN through the generation of NO and the subsequent conversion of NO to

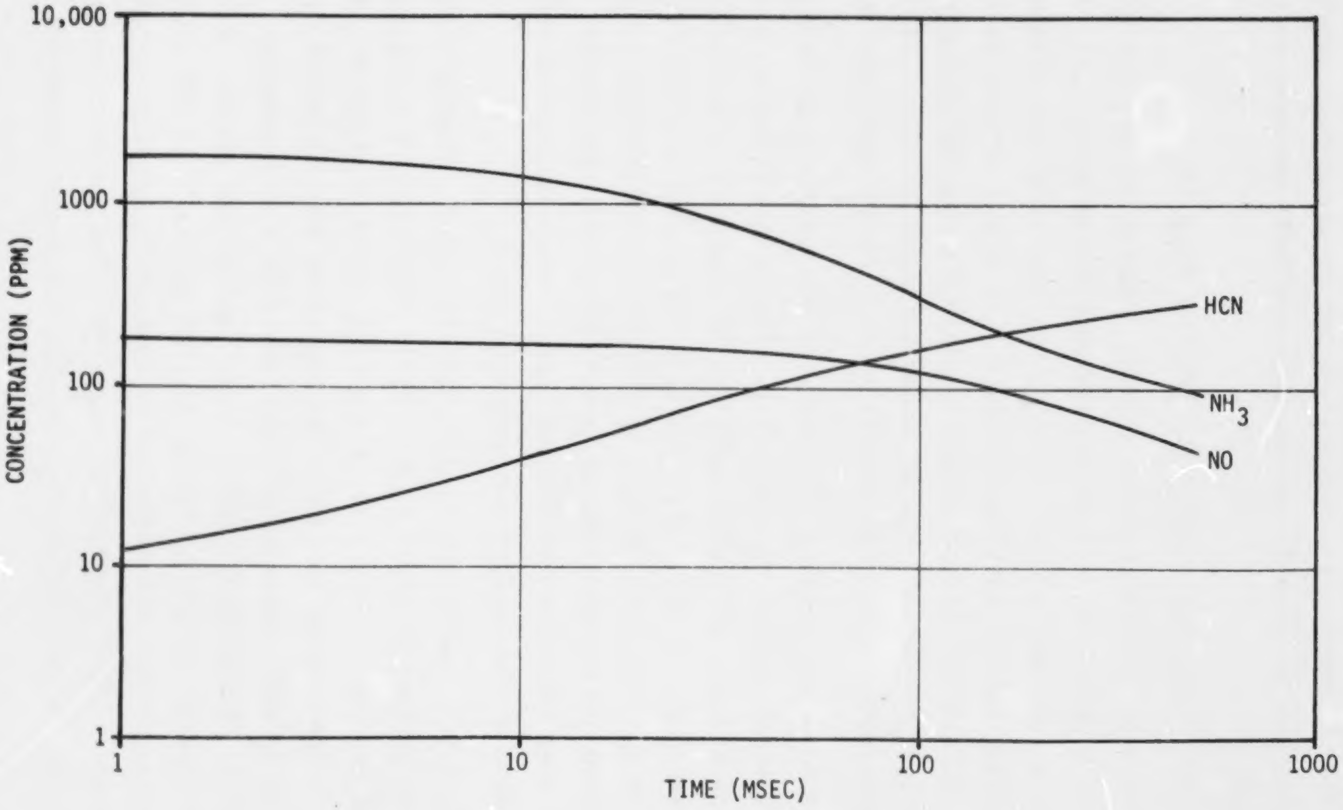


Figure 4-12. Nitrogen Species from Premixed Rich Primary Zone — Adiabatic Gas Turbine Combustor

NOTE: $\phi = 2.0$; $T_{outlet} = 2955^{o}F$; Coordinate values from stirred reactor zone $\tau_{SR} = 1$ msec; LOG/LOG coordinates; $NH_3 = 4000$ ppm in fuel

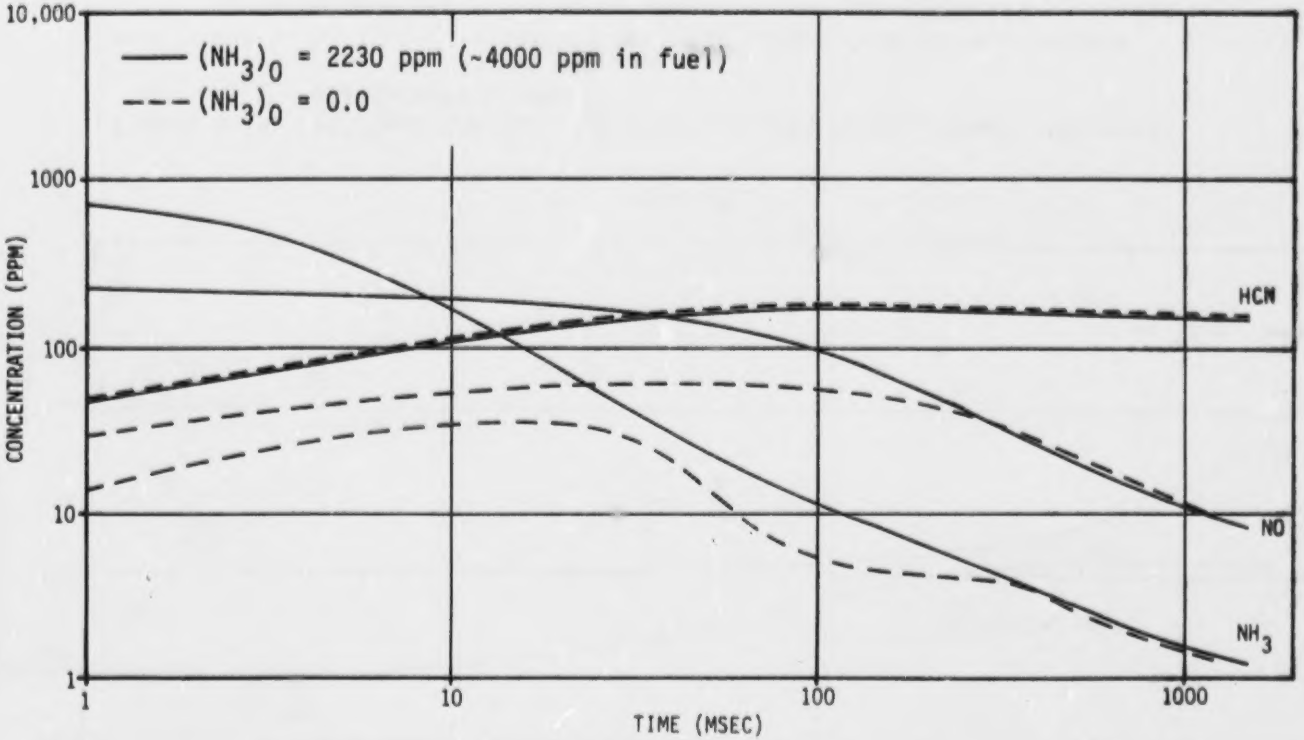


Figure 4-13. Nitrogen Species from Premixed Rich Primary Zone – Adiabatic Gas Turbine Combustor

NOTE: $\phi = 1.67$; $T_{outlet} = 3167^{o}F$: Ordinate values from reactor ignition zone $\tau_{SR} = 1.0$ msec; LOG/LOG coordinates

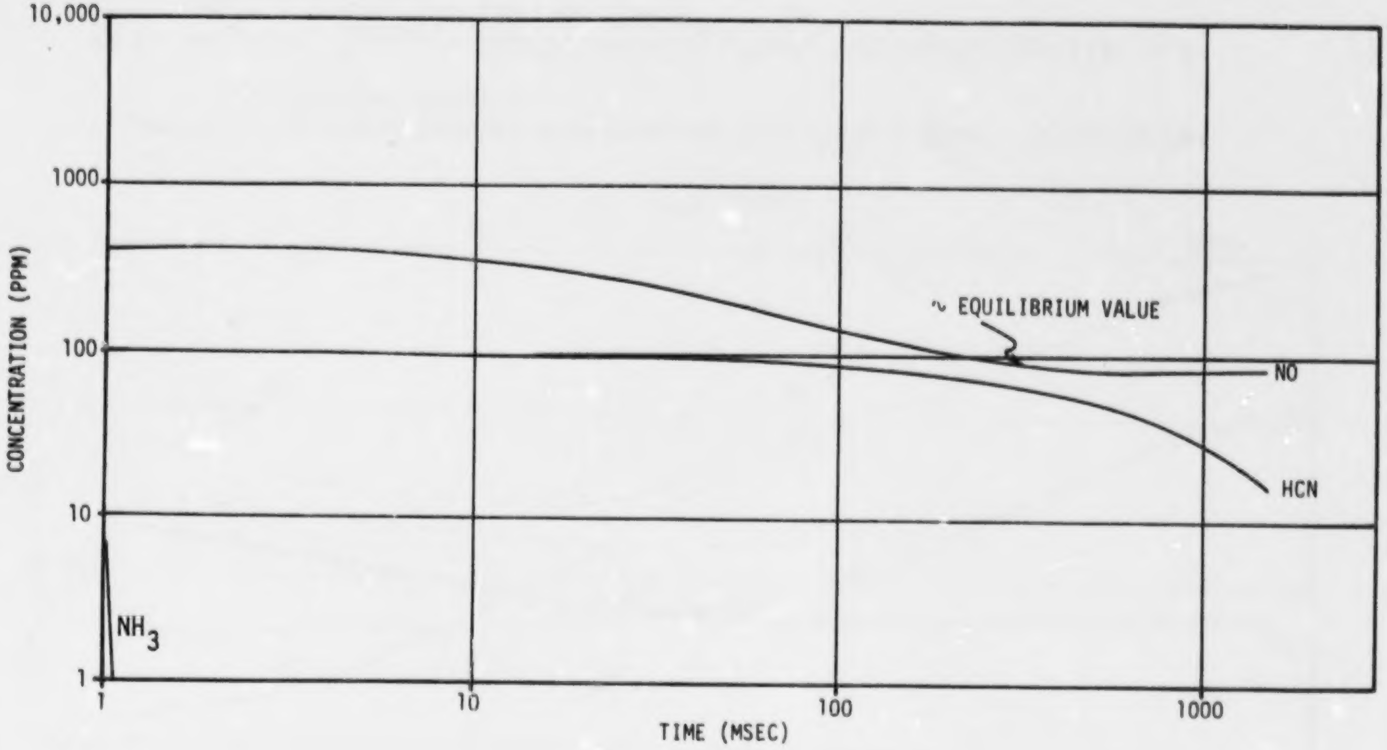


Figure 4-14. Nitrogen Species from Premixed Rich Primary Zone — Adiabatic Gas Turbine Combustor

NOTE: $\phi = 1.33$; $T_{outlet} = 3475^{o}F$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; $(NH_3)_0 = 2005$ ppm (4000 ppm in fuel); LOG/LOG coordinates

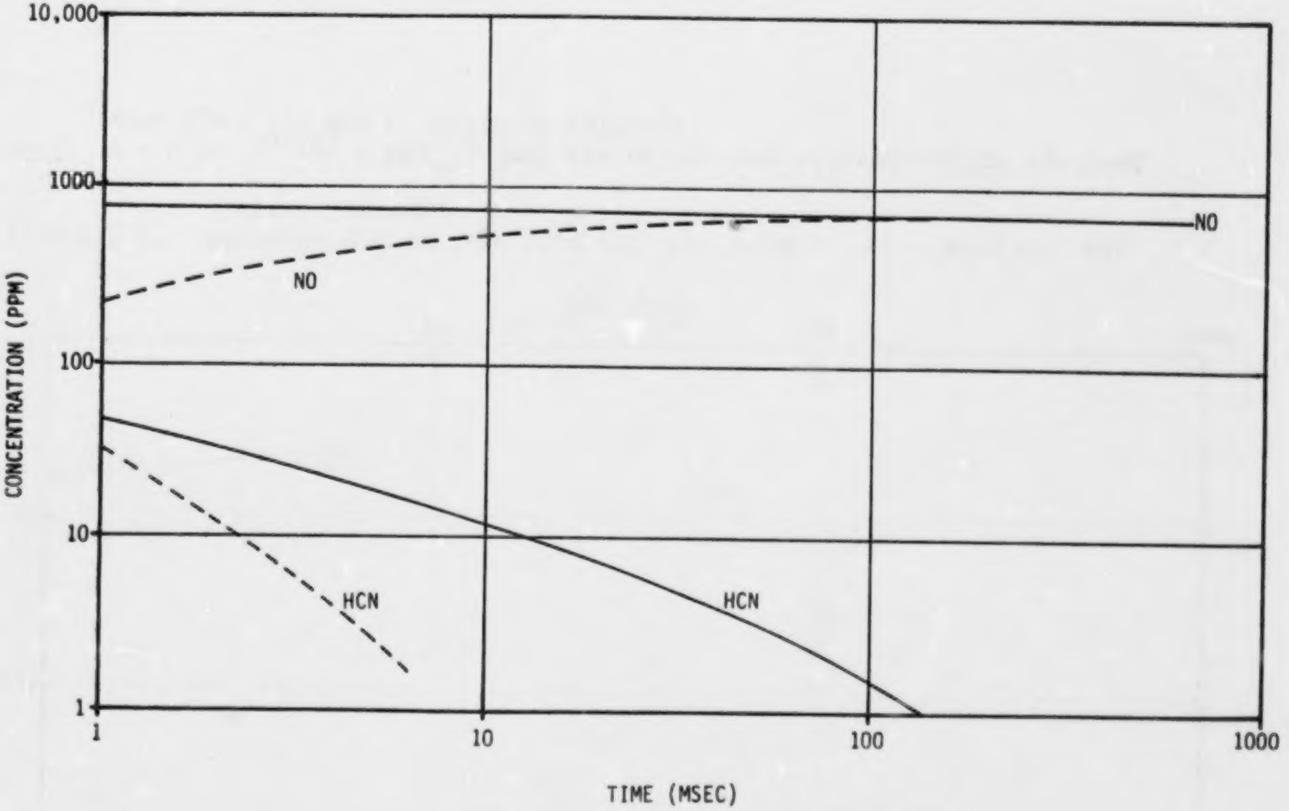


Figure 4-15. Nitrogen Species from Rich Primary Zone — Adiabatic Gas Turbine Combustor

NOTE: $\phi = 1.1$; $T_{outlet} = 3650^{o}F$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; LOG/LOG coordinates; $NH_3 = 4000$ ppm in fuel

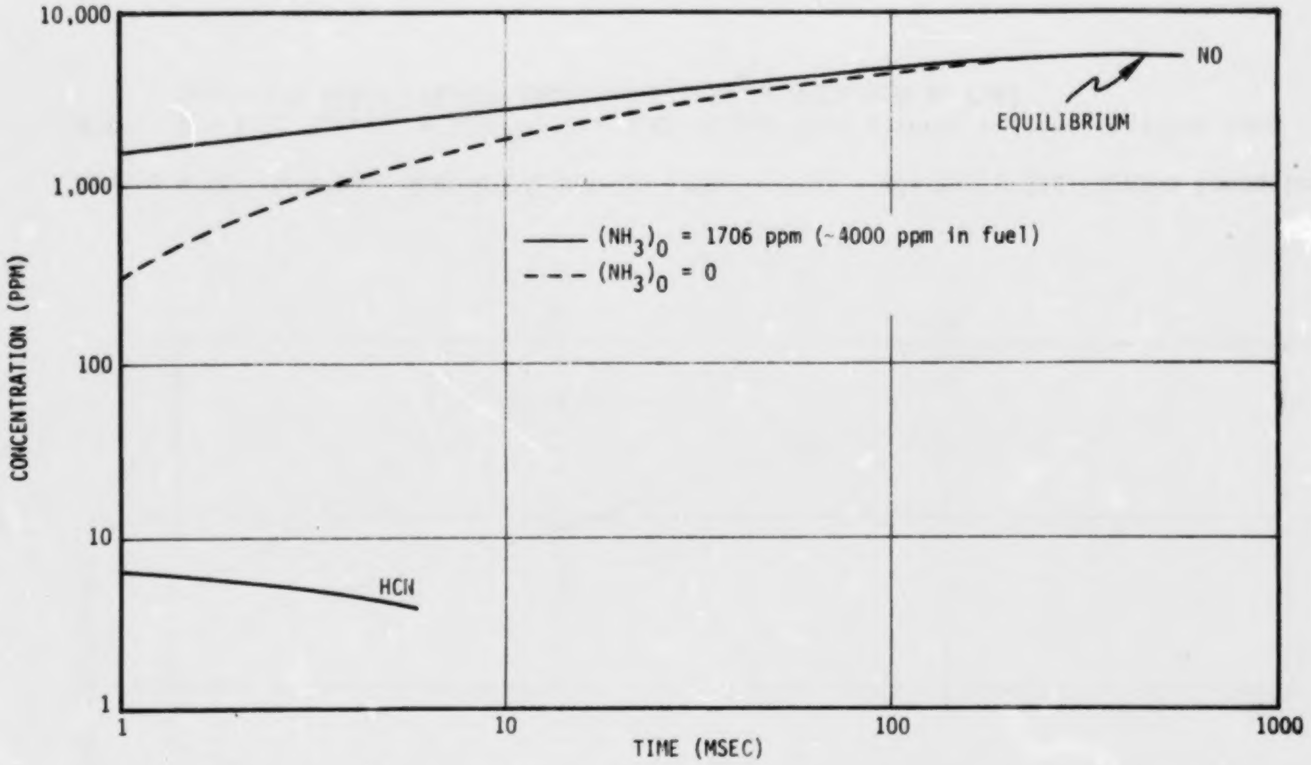


Figure 4-16. Nitrogen Species from Premixed Lean Primary Zone — Adiabatic Gas Turbine Combustor

NOTE: $\phi = 0.9$; $T_{outlet} = 3600^{o}F$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; LOG/LOG coordinates

HCN through the Myerson reaction is also a possibility although the NO levels, and hence, the reaction rates are low. Again, these comments must be taken as speculative since the HCN production and destruction reactions are poorly understood under rich conditions.

Figure 4-13 shows the results for the ϕ=1.67 case. Approximately 50 percent of the fuel NH_3 has converted to N_2 within the stirred reactor. Appreciable "prompt" NO and HCN are generated and NO decays slowly toward equilibrium. Superequilibrium HCN synthesis continues during the first 100 ms of the primary zone. After 100 msec the HCN concentration becomes frozen, indicating that the decomposition reactions are either very slow or improperly modeled.

Initial Fuel Ammonia Content

Figure 4-13 also shows the behavior for the ϕ=1.67 case in the absence of any fuel ammonia. All of the NO precursors, HCN, NH_3, and NO itself experience prompt synthesis in the stirred reactor which is continued during the first 30 msec of the plug flow. The HCN generation is identical to that with fuel nitrogen present indicating that the mechanism is entirely Fenimore. The NO generation is apparently also due to the Fenimore mechanism of N atom generation followed by the modified Zeldovich reactions. When the N atom production ceases due to a decay in hydrocarbon radicals, the HCN freezes and the NO commences its decay to equilibrium. The NH_3 synthesis again apparently rests on the N atom generation. It is speculated that the dominant generation mechanism is

$$N + OH \rightarrow NH + O$$

$$NH + OH \rightarrow NH_2 + O$$

$$NH_2 + OH \rightarrow NH_3 + O$$

Again, when the N atom production ceases the NH_3 starts to decay towards equilibrium. Surprisingly this final reduction of NO and NH_3 towards equilibrium becomes identical with that for the case with fuel nitrogen present.

The results for ϕ=1.33 are shown in Figure 4-14. The fuel NH_3 essentially vanishes completely within the stirred reactor with two-thirds of the N appearing as N_2. Of the remaining portion most is manifested as NO with about 100 ppm of HCN. The NO and HCN decay very slowly towards their equilibrium states with the NO reaching that value (90 ppm) in approximately 200 msec. At this point 60 ppm of HCN still remains yielding a total amount of NO precursors of 8 percent of the initial level of NH_3. Such a result certainly must be considered encouraging provided a practical combustor design can be evolved with primary zone residence times in excess of 100 msec.

In Figure 4-15 the results for ϕ=1.1 are presented. This case is clearly too lean with only about 50 percent of the fuel nitrogen promptly converted to N_2. The remaining portion is primarily converted to NO within the stirred reactor at a level of 900 ppm which is approximately the equilibrium value. 50 ppm of prompt HCN decays to zero in approximately 100 msec probably through reactions with OH to form CN. In comparison with the undoped case the HCN decay is quite slow. This may be a consequence of a HCN production contribution through the Myerson reaction due to the high initial NO levels in the case with fuel nitrogen present. The influence of initial level of NH_3 is felt only for the first 100 msec after which the system is equilibrated. The results for ϕ=0.9 are included in Figure 4-16 for completeness. They are similar in nature to the ϕ=1.1 case with equilibration occurring within 100 msec.

In Figure 4-17 the adiabatic plug flow primary zone results are compiled in a different manner where the sum of the mole fractions of the nitrogen-containing species (not including N_2) normalized by the initial $(NH_3)_0$ mole fraction are plotted as a function of ϕ for various residence times. On the lean side, thermal NO production dominates with peak values occurring at approximately ϕ=0.9. On the rich side the residual nitrogen fraction has a minimum at an equivalence ratio around 1.4 and the magnitude of this fraction decreases with time, reaching a value of 0.10 at t=200 msec.

Air Nitrogen Replaced by Argon

In order to assess the importance of N_2 content, a set of calculations was conducted with the nitrogen content of the air replaced by an equal mole fraction of argon. The mixture (O_2-Ar) temperature was adjusted to yield the

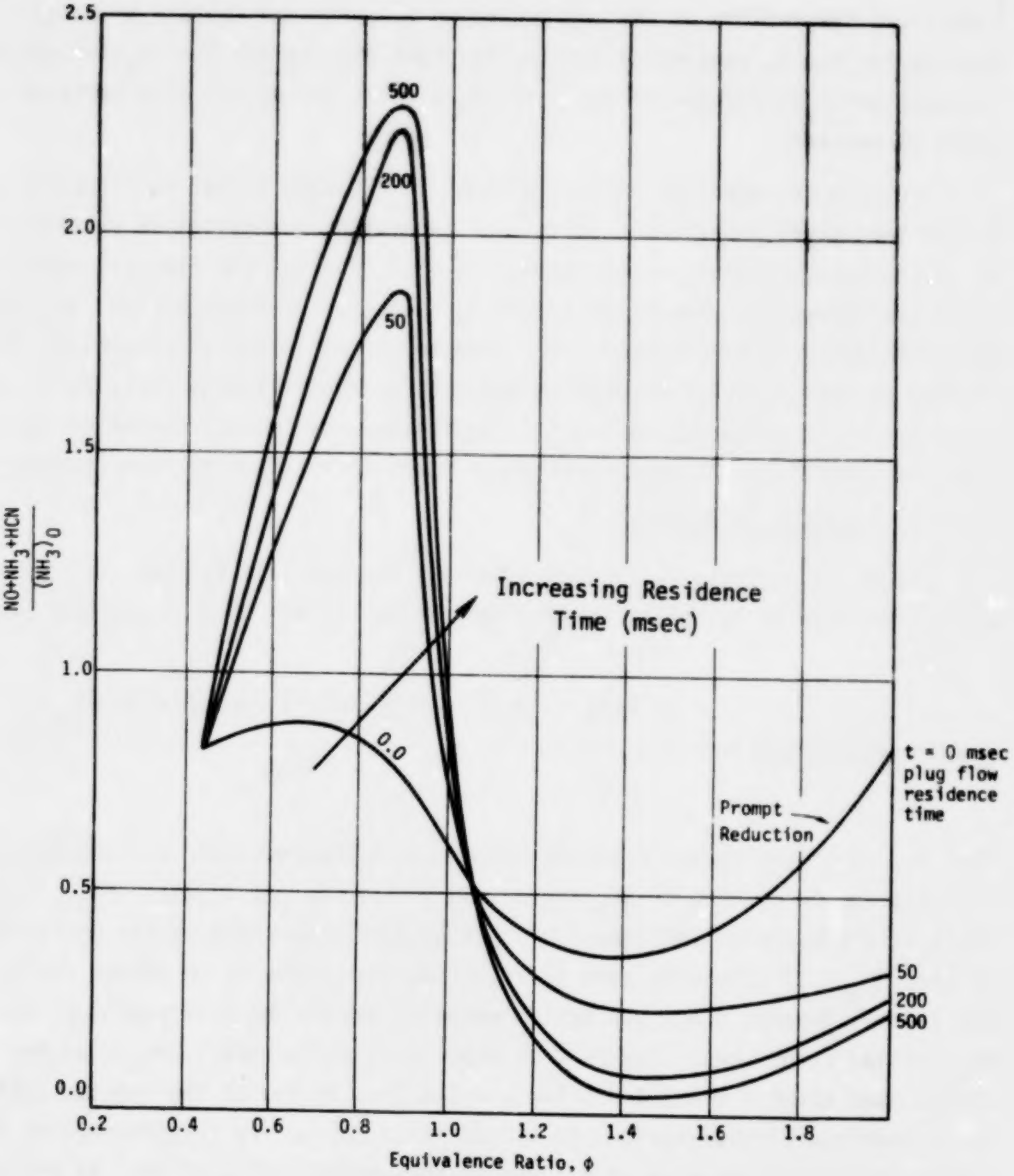


Figure 4-17. Sum of Residual Nitrogen Species from Premixed Plug Flow Primary — Adiabatic Gas Turbine Combustor

NOTE: T_{air} = 1000°F; T_{fuel} = 1500°F; P = 10 atm; τ_{SR} = 1 msec (ignition); NH_3 = 4000 ppm in fuel same flame temperature as the corresponding low Btu fuel gas/air mixture. Considering the N_2 content of the low Btu fuel gas, at $\phi=1$ the (O_2-Ar) system replaces about 70 percent of the total N_2 with Ar and at $\phi=0.5$ it replaces about 80 percent.

Figure 4-18 shows the results plotted in the same format as Figure 4-17. On the lean side there is a reduction of thermal NO generation in proportion to the N_2 concentrations as expected. On the rich side the Fenimore reaction rates are reduced in proportion to the N_2 reduction, and hence, HCN, NH_3 and NO generations are all reduced. For example, at $\phi=1.4$ and t=50 msec, N_2 is reduced by approximately 60 percent and the residual nitrogen fraction is cut by more than 50 percent, showing the significance of the N_2 content on the rich side behavior. At larger residence times this effect is less pronounced.

Summary of Results

Figure 19 presents the Premixed Primary Reactor data for LBG fuel gas and air in the form of an "effective NH_3 conversion ratio" which is defined by:

$$\text{effective } NH_3 \text{ conversion ratio} = \frac{\left\{[NO] + [NH_3] + [HCN]\right\} - \left\{[NO] + [NH_3] + [HCN]\right\}_{(NH_3)_0 = 0}}{(NH_3)_0}$$

That is, it is the excess nitrogen-containing molecules, over and above those existing in the absence of NH_3 doping, normalized by the initial $(NH_3)_0$. This ratio is a measure of additional N-containing molecules due to the presence of initial NH_3. If it equals zero it signifies that there is no effect due to the initial doping, i.e., the system behavior has become independent of the NH_3 initial conditions. Figure 4-19 shows that these conditions occur for $t \geq 200$ msec and $0.8 < \phi < 1.7$. For $\phi < 1.1$ this is due to the reactor achieving a near-equilibrium state. At $\phi=1.33$ it is due to the independence of HCN production on the presence of NH_3 and to the equilibration of NO. At $\phi=1.67$ Figure 4-13 previously demonstrated that the concentrations for the ammonia-doped and undoped cases merge at t=200 msec. Again the HCN production is independent of $(NH_3)_0$. In the absence of initial ammonia, NO is produced via N generation by the Fenimore reactions. NH_3 is synthesized in a similar manner in the absence of initial doping by a chain which is initiated by N and NH

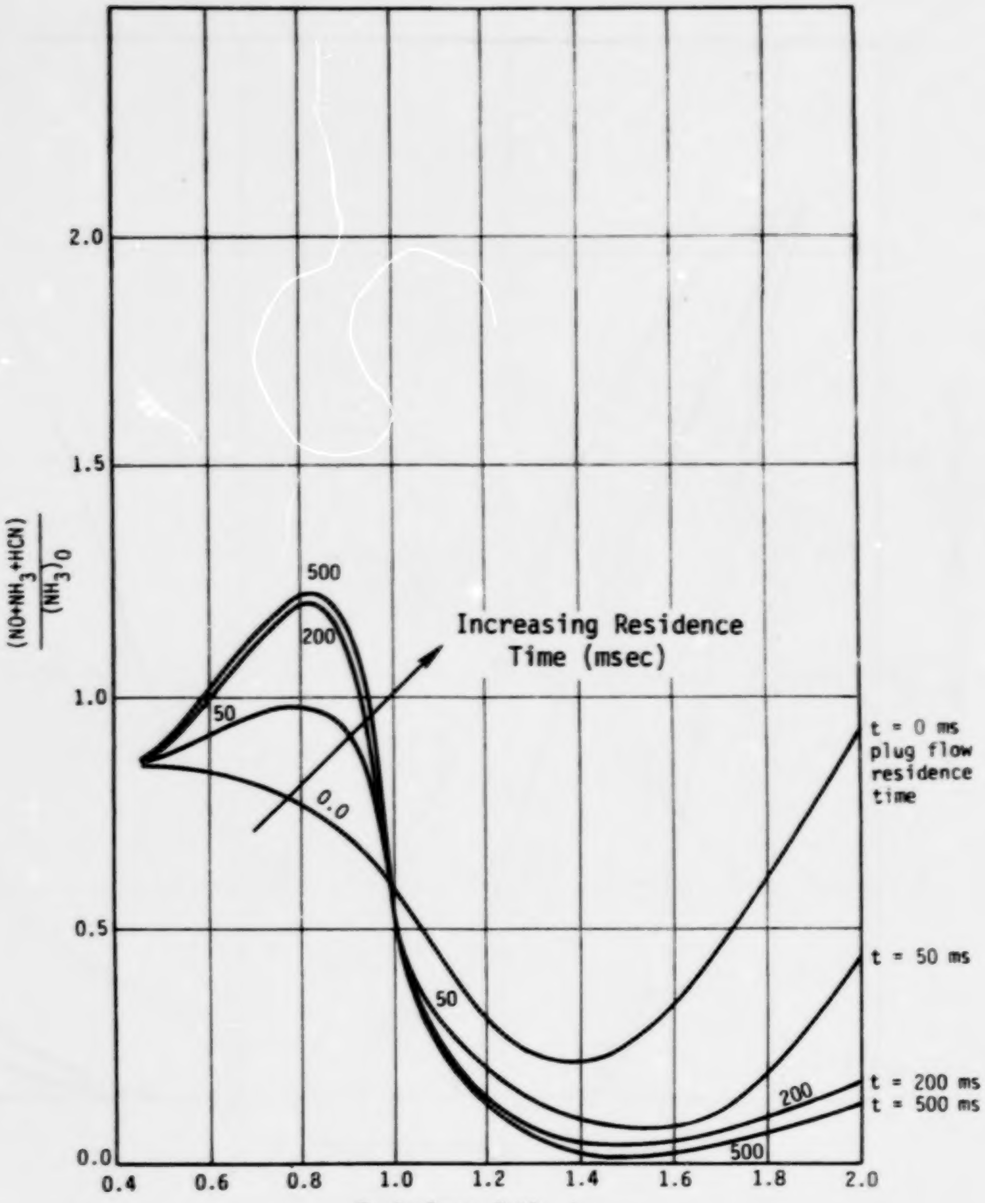


Figure 4-18. Sum of Residual Nitrogen Species from Premixed Plug Flow Primary — Adiabatic Gas Turbine Combustor — N_2 in Air Replaced by Argon

NOTE: $T_{(O_2\text{-}Ar)}$ is adjusted such that flame temperature is same as for Air; T_{fuel} = 1500°F; P = 10 atm; τ_{SR} = 1 ms; $(NH_3)_{fuel}$ = 4000 ppm; $[AR]/[O_2]$ = 3.79 (same as for air)

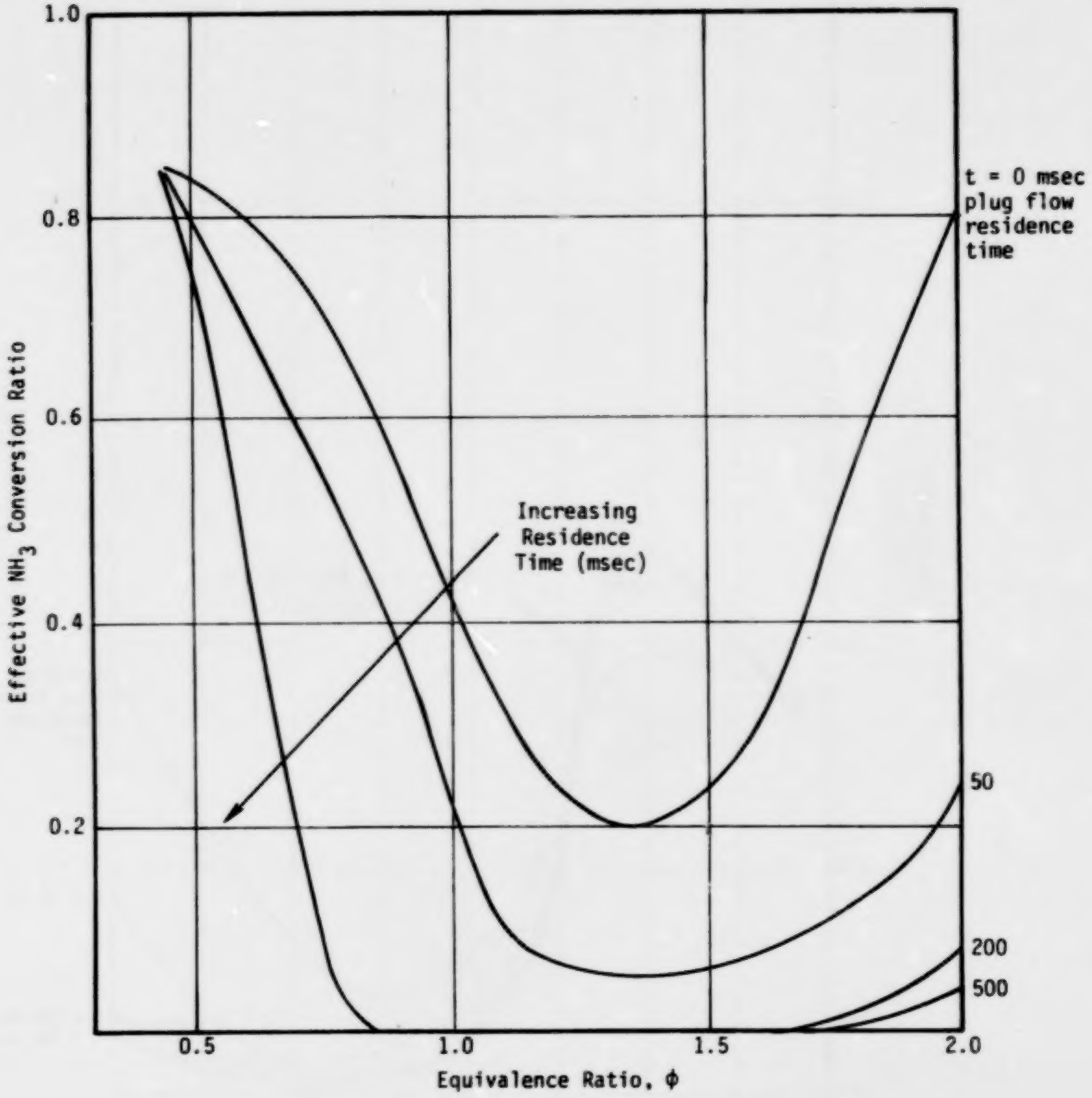


Figure 4-19. Effective (NH_3) Conversion Ratio for Premixed Rich Primary Reactor — Adiabatic Gas Turbine Combustor

NOTE: P = 10 atm; τ_{SR} = 1 msec (ignition); NH_3 = 4000 ppm in fuel; T_{air} = 1000°F; T_{fuel} = 1500°F production through the Fenimore reactions. Both NO and NH_3 so generated eventually reach the levels associated with NH_3 doping, and therefore, follow the same decay behavior.

In summary, a baseline rich primary reactor burning fuel containing 4000 ppm NH_3 with $1.33 < \phi < 1.45$ designed for a residence time on the order of 200 msec will have a residual nitrogen species concentration of less than 200 ppm. This appears to be near the optimum design point without requiring excessive residence times.

4.3.3.3 Deviations from Baseline Primary Reactor Specifications

Now that the factors influencing NO_x production in the baseline primary reactor have been discussed, the following additional variables will be addressed:

- Heat transfer from plug flow reactor
- Stirred reactor residence time
- Pressure
- Fuel composition - methane content

Heat Transfer Effects

Heat transfer effects were examined by comparing the nitrogen-bearing species time histories for the adiabatic case with those for an instantaneous heat removal equivalent to a temperature drop of 267°F. The effect of heat extraction from the rich primary zone depends on when the heat transfer takes place. Figure 4-20 shows the results for the ϕ=1.67 case with early heat removal immediately following the stirred reactor zone (1.0 ms). The effect is to reduce all of the reaction rates which results initially in a retardation of the decay of the cumulative NO precursors. After long periods, however, the effect of cooling appears to be small. Figure 4-21 indicates that taking the same amount of heat out late in the process (t=500 ms) has essentially no effect. Figure 4-22 shows the effect of early cooling (after 1.0 ms) for ϕ=1.33. The heat transfer here was increased to produce a 475°F temperature reduction to further emphasize the effects. In this case the reduction in temperature is sufficiently great to freeze the HCN at its initial level and to retard the

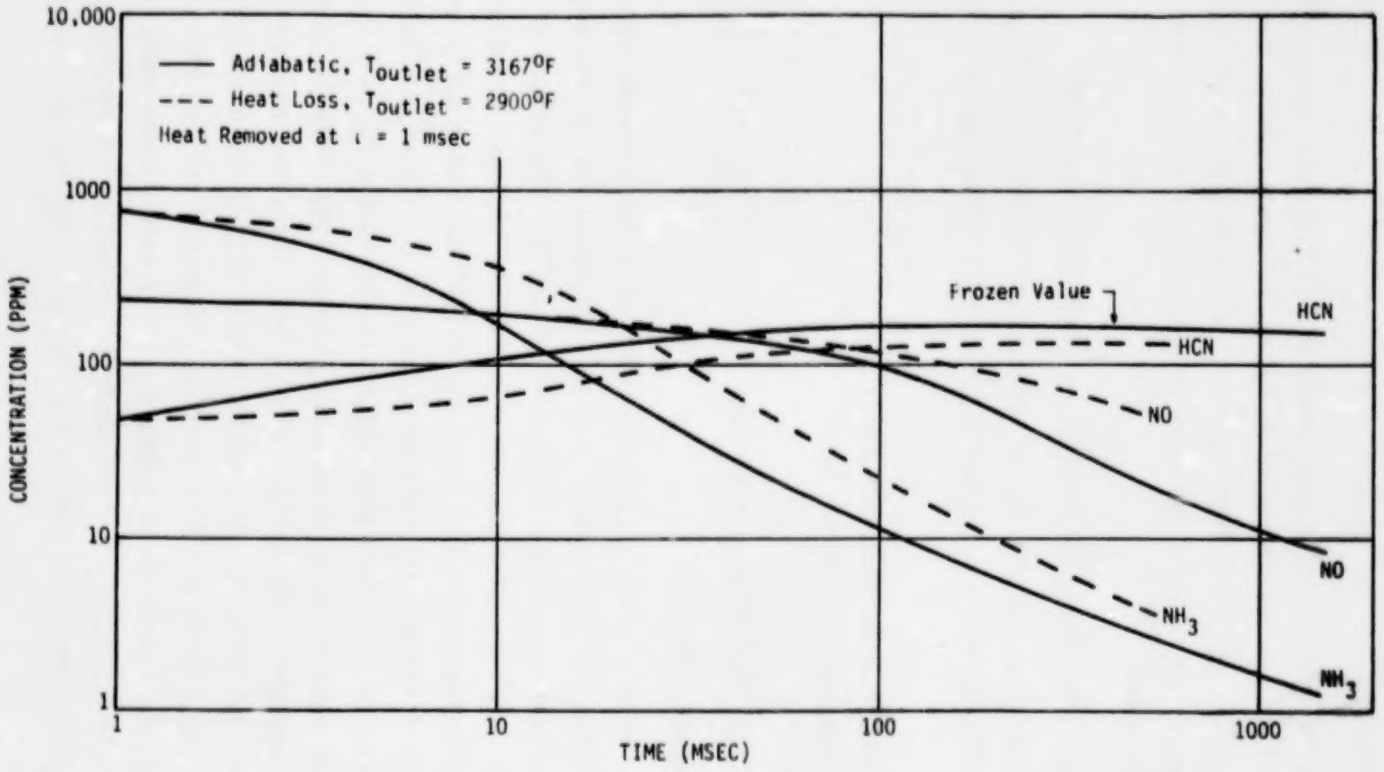


Figure 4-20. Nitrogen Species from Rich Primary Zone with Early Heat Removal — Adiabatic Gas Turbine Combustor

NOTE: $\phi = 1.67$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1$ msec; $[HCN]_{eq} < 5$ ppm; $(NH_3)_0 = 2230$ ppm (~4000 ppm in fuel); LOG/LOG coordinates

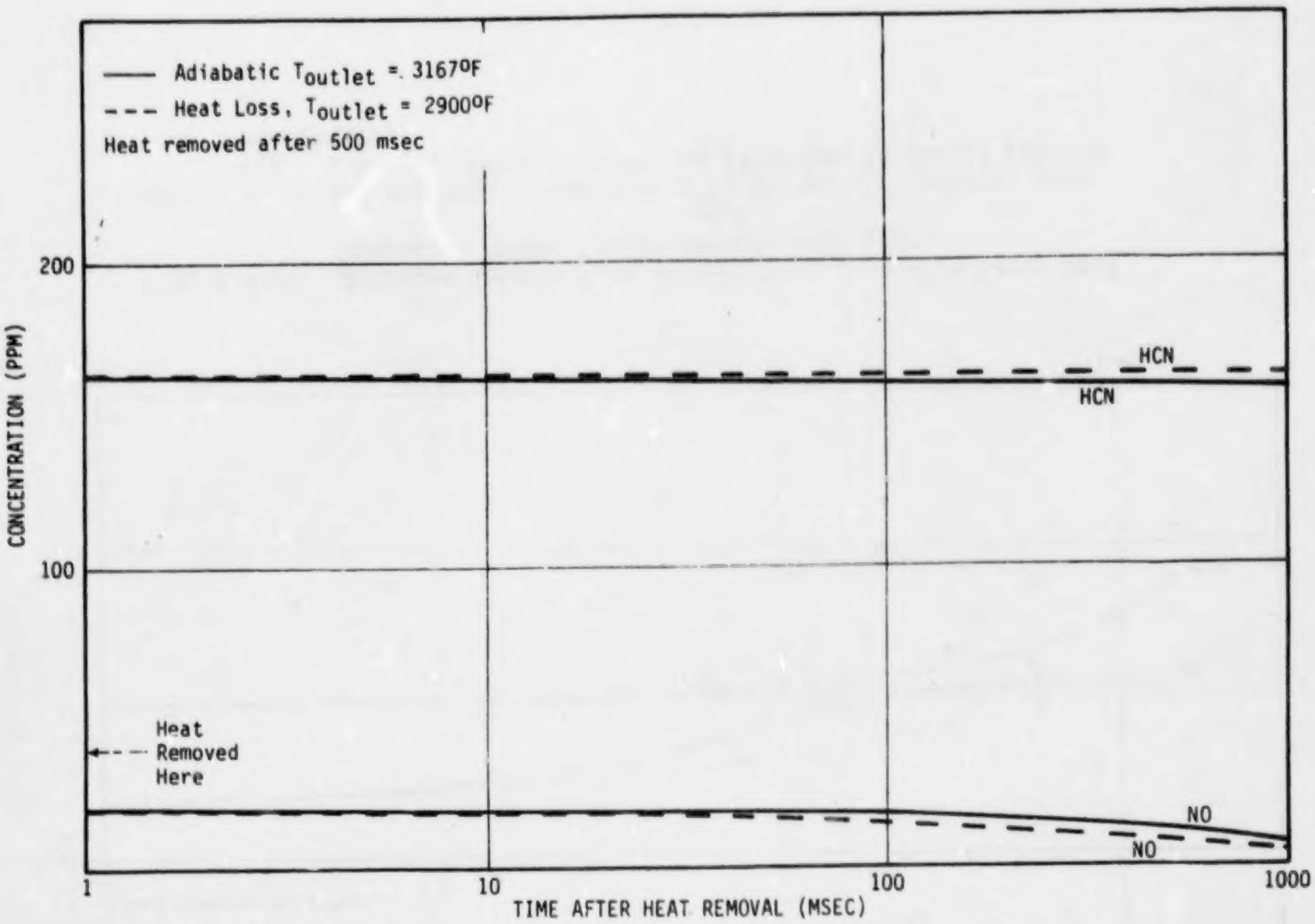


Figure 4-21. Nitrogen Species from Rich Primary Zone with Late Heat Removal — Adiabatic Gas Turbine Combustor

NOTE: ϕ = 1.67; Ordinate values from uncooled plug flow zone, τ_{SR} = 500 ms; $(NH_3)_0$ = 2230 ppm (~4000 ppm in fuel); $(HCN)_{eq}$ = 5 ppm; LOG/LOG coordinates

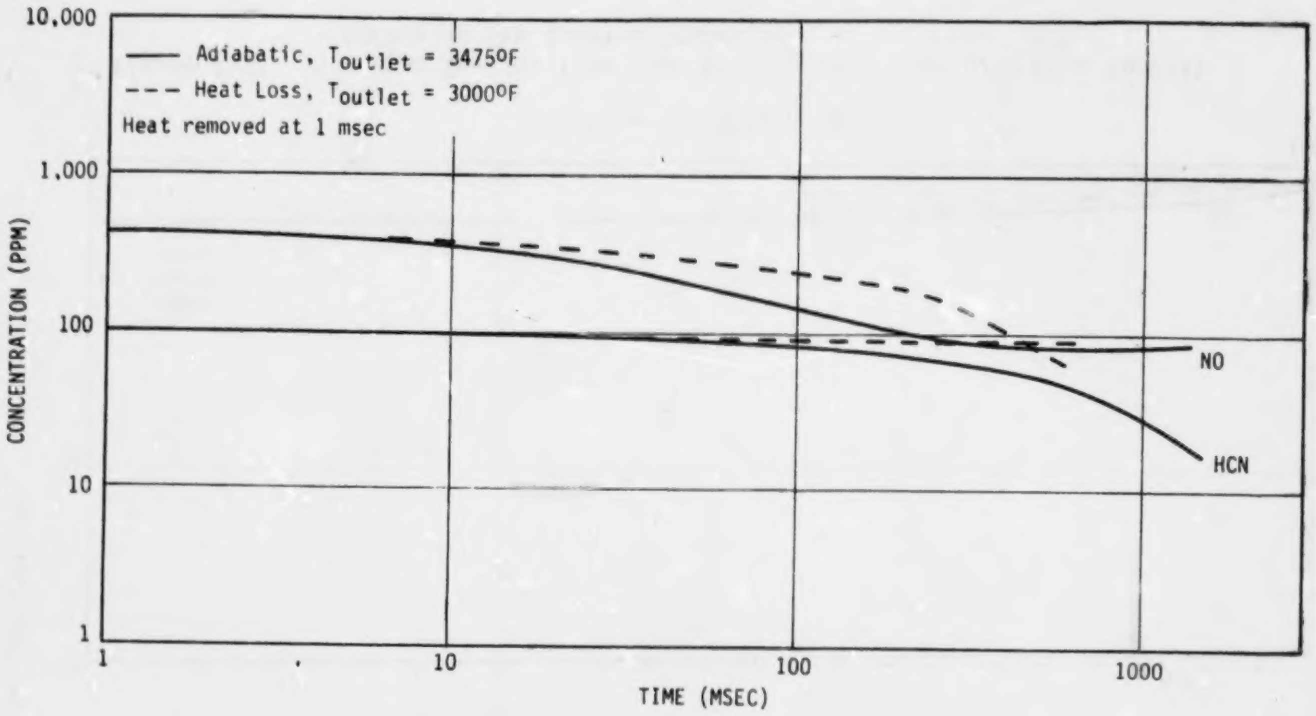


Figure 4-22. Nitrogen Species from Rich Primary Zone with Early Heat Removal — Adiabatic Gas Turbine Combustor

NOTE: ϕ = 1.33; Ordinate values from stirred reactor ignition zone τ_{SR} = 1.0 msec; $(NH_3)_0$ = 2005 ppm (4000 ppm in fuel); LOG/LOG coordinates decay of NO. The combined NO and HCN remain high until t=500 ms when the trend is reversed due to the NO seeking a lower equilibrium value. Figure 4-23 indicates that cooling late in the process (t=500 ms) for ϕ=1.33 yields a lower combined NO and HCN due to the NO seeking a lower equilibrium value. Such late cooling is, of course, unrealistic and is included here only to provide insight into primary zone behavior.

Stirred Reactor Residence Time Effects

Figure 4-24 presents an extreme case in which the entire ϕ=1.33 primary reactor is taken to be well-stirred with a residence time of 500 msec. The effect is to produce a system which appears much richer than the corresponding plug flow. CH and CH_4 concentrations are higher than the plug flow by a factor of 10^4. Further, the stirred reactor has lower O, OH and H by a factor of 2. The net result is that the long residence time stirred reactor has much higher HCN and somewhat higher NO levels than the corresponding plug flow reactor.

In Figure 4-25 the effect of stirred reactor residence time for a lean situation (ϕ=0.9) is examined. Stirred reactors with residence times of 0.5, 1.0, and 5.0 msec were followed by plug flow reactors. The concentrations, when plotted again total stirred and plug flow reactor residence time, show no effect of this variation.

Pressure Effects

Figure 4-26 illustrates the effect of pressure reduction for the ϕ=1.33 case. An extreme example was chosen (P=1 atm) in order to emphasize the effect. In comparison with the 10 atmosphere case (also plotted), the NO level increases and the HCN level decreases as pressure is reduced. The increase in NO level is consistent with the increase of equilibrium NO concentrations with reduction in pressure under rich conditions due to the increase in equilibrium oxygen concentration as the pressure drops. The Fenimore HCN production rate is expected to be roughly proportional to pressure.

Figure 4-27 shows similar results for reduced pressure at ϕ=0.9. For lean conditions there is little pressure effect since equilibrium NO concentrations are pressure-independent on the lean side.

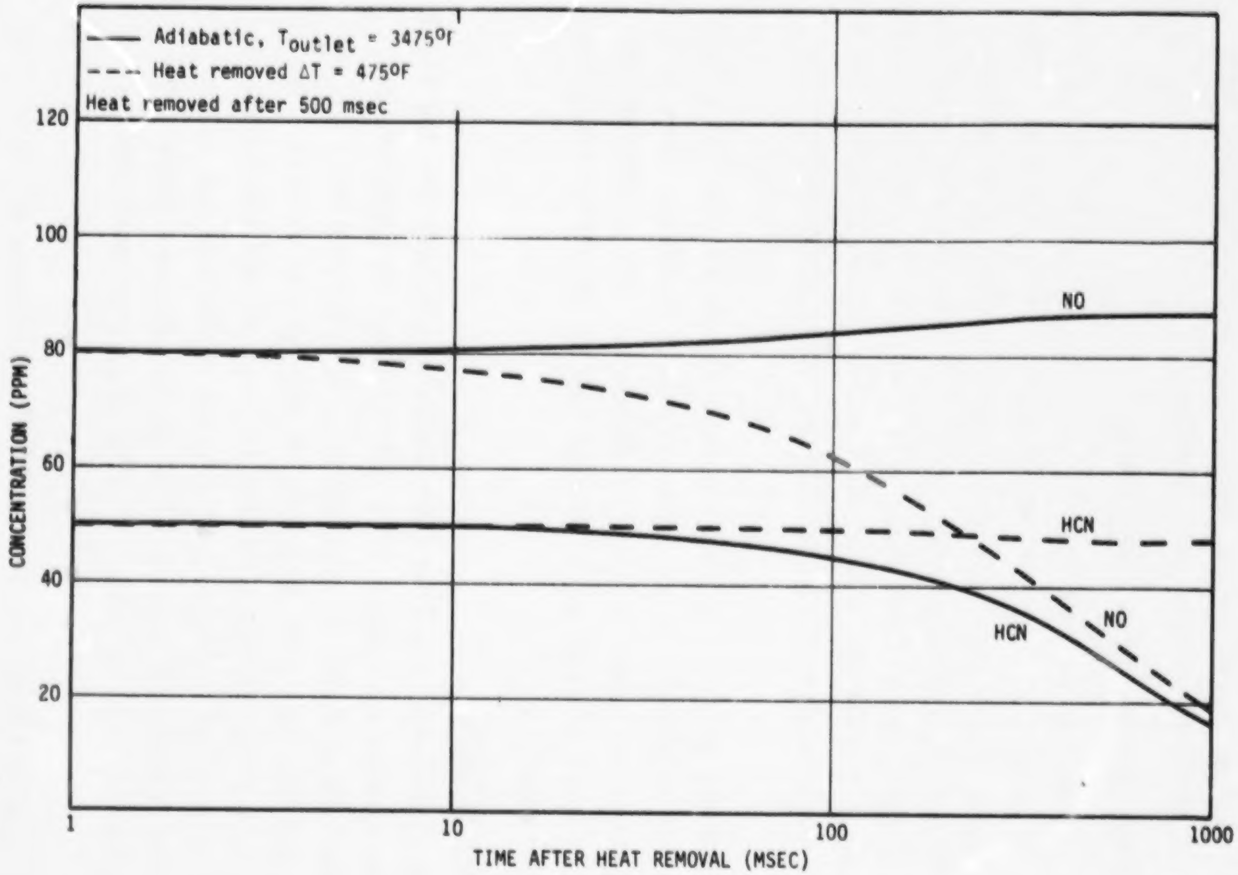


Figure 4-23. Nitrogen Species from Rich Primary Zone with Late Heat Removal — Adiabatic Gas Turbine Combustor

NOTE: ϕ = 1.33; Ordinate values from uncooled plug flow zone, τ_{SR} = 500 ms; $(NH_3)_0$ = 2005 ppm (4000 ppm in fuel); Log time coordinate; $(HCN)_{eq} < 5$ ppm

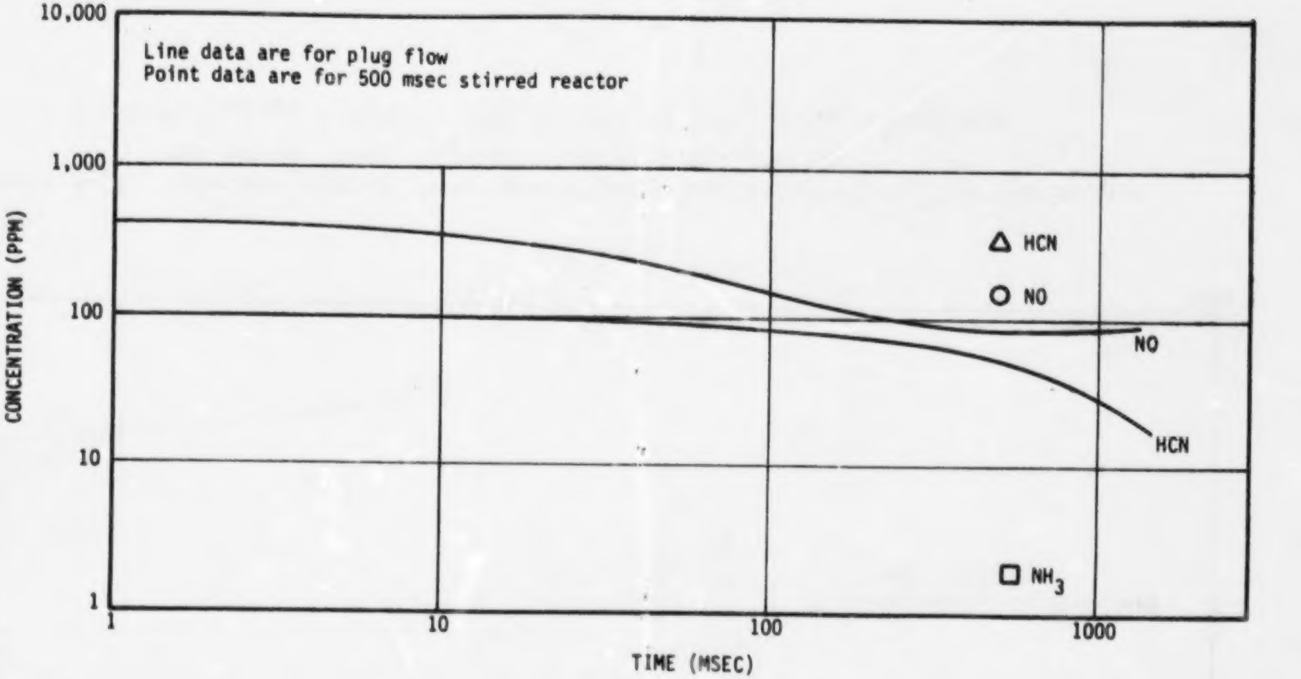


Figure 4-24. Nitrogen Species from Rich Primary Zone, Stirred/Plug Flow Comparison — Adiabatic Gas Turbine Combustor

NOTE: $\phi = 1.33$; $T_{outlet} = 3475^{o}F$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1$ msec; $(NH_3)_0 = 2005$ ppm (4000 ppm in fuel); No heat transfer; LOG/LOG coordinates

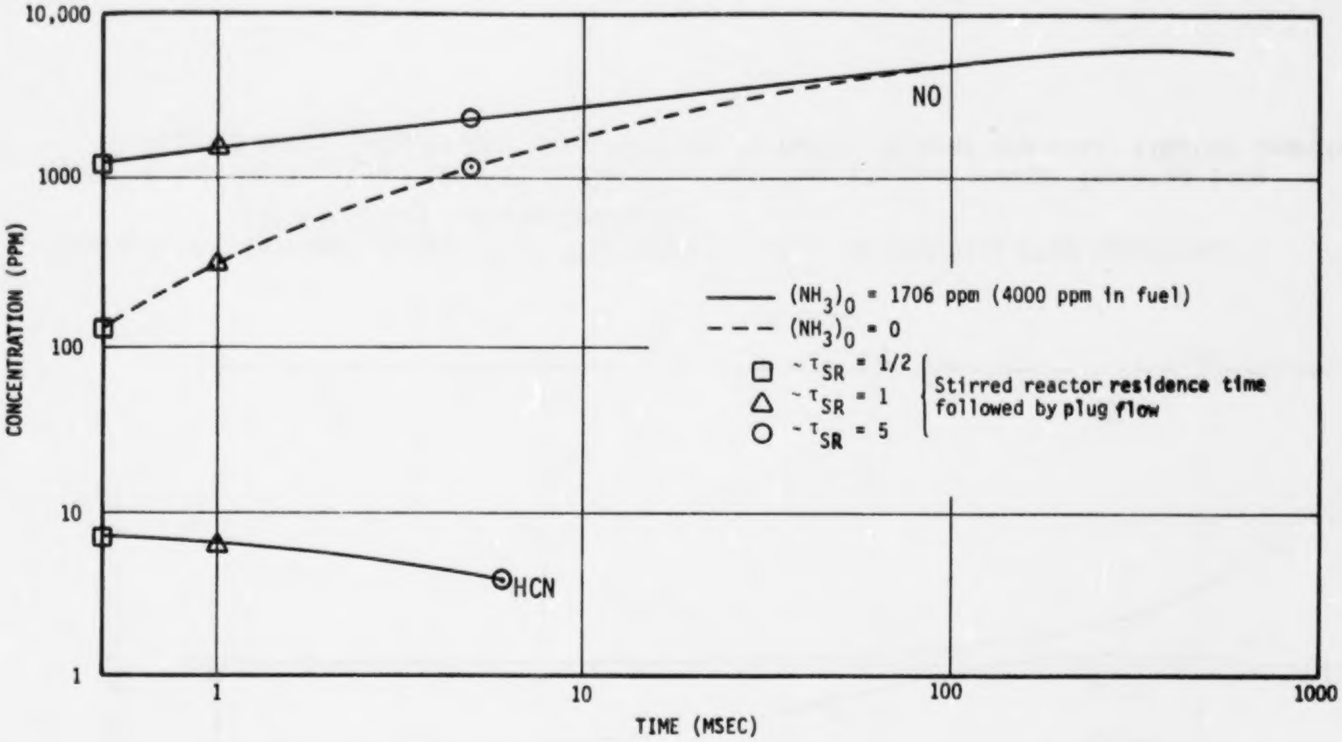


Figure 4-25. Nitrogen Species from Lean Primary Zone with Varying Stirred Reactor Residence Time — Adiabatic Gas Turbine Combustor

NOTE: $\phi = 0.9$; $T_{outlet} = 3600^{o}F$; LOG/LOG Coordinates; $(NO)_{eq} = 3680$ ppm

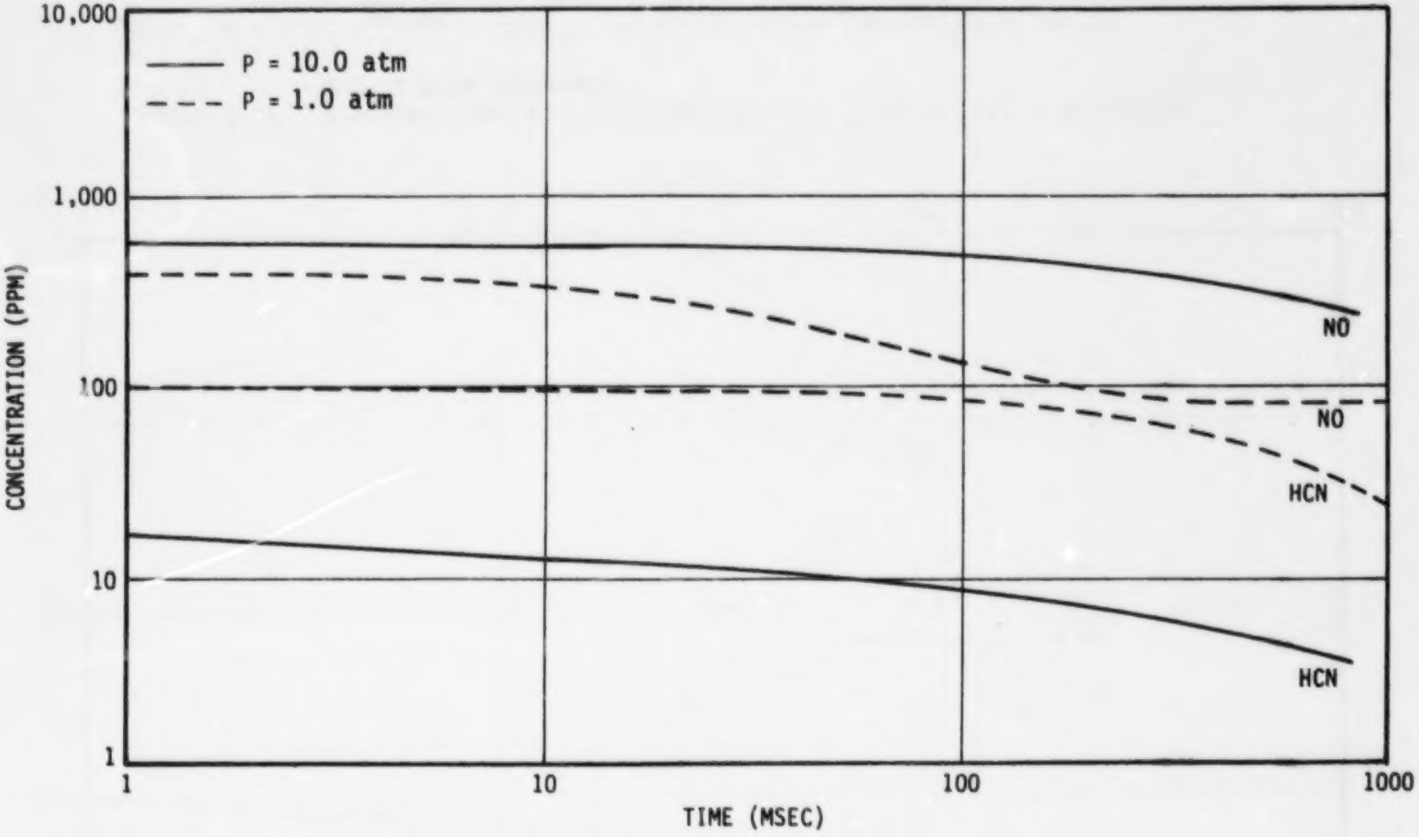


Figure 4-26. Nitrogen Species from Premixed Rich Primary Zone — Adiabatic Gas Turbine Combustor — Effect of Pressure

NOTE: $\phi = 1.33$; $T_{outlet} = 3475^{o}$; Ordinate values from stirred reactor ignition zone τ_{SR} = 1 msec; $(NH_3)_0$ = 2005 ppm (4000 ppm in fuel); LOG/LOG coordinates

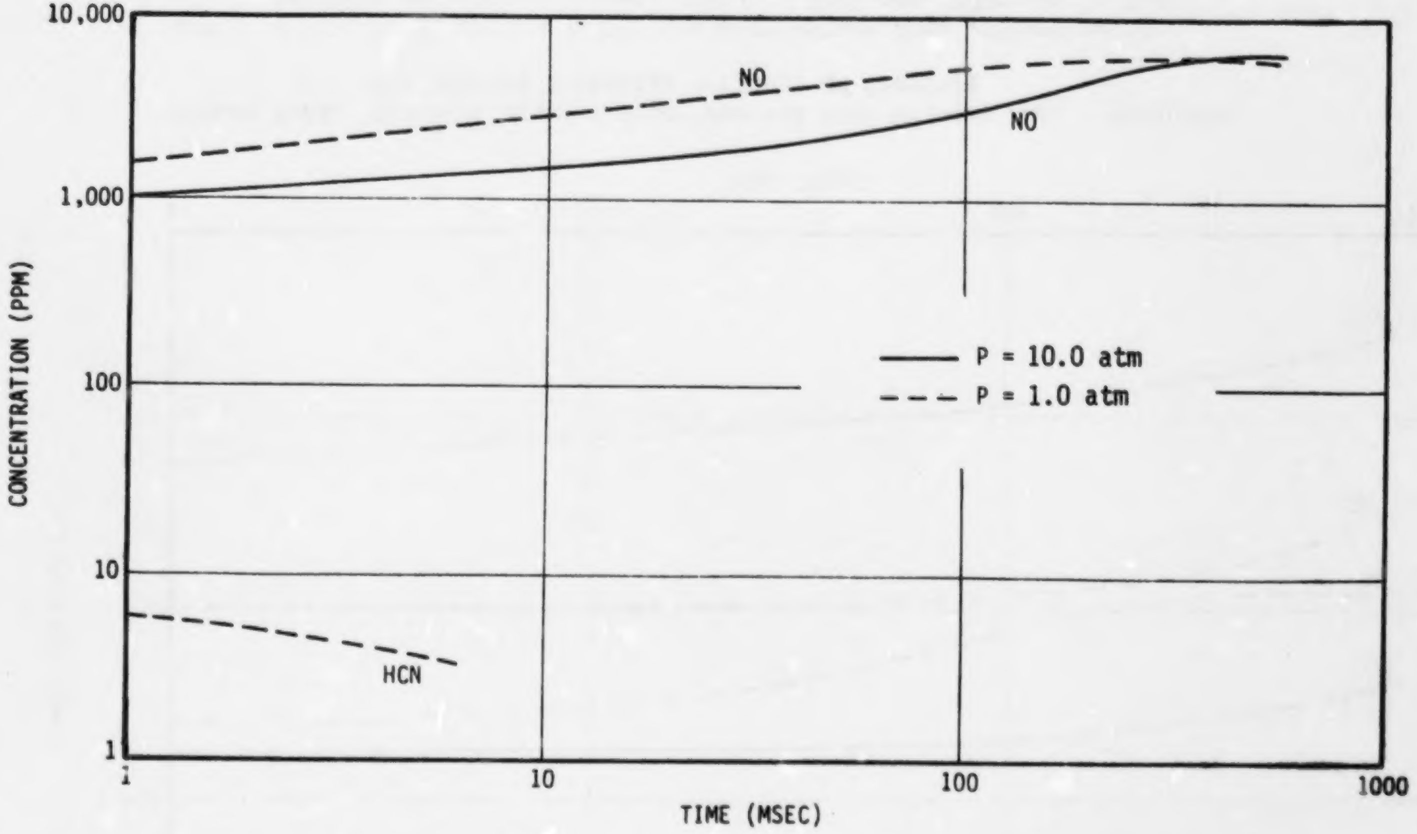


Figure 4-27. Nitrogen Species from Premixed Lean Primary Zone — Adiabatic Gas Turbine Combustor

NOTE: $\phi = 0.9$; $T_{outlet} = 3600^{o}F$; Ordinate values from stirred reactor ignition zone τ_{SR} = 1 msec; $(NH_3)_0$ = 1706 ppm (4000 ppm in fuel); LOG/LOG coordinates

Fuel Composition Effect

The effect of fuel methane content was simulated by replacing the methane with CO and H_2 such that the overall C/H ratio, equivalence ratio, and enthalpy remained unchanged. This is equivalent to allowing the hypothetical reaction

$$CH_4 + 1/2\ O_2 \rightarrow CO + 2H_2$$

to proceed instantaneously. Figure 4-28 compares the results for ϕ=1.33 with and without methane. The absence of hydrocarbon fragments eliminates the Myerson and Fenimore-type reactions, and hence, HCN is absent in Figure 4-28. The NO level is only slightly affected showing a somewhat higher level in the absence of the Myerson decay mechanism and the Fenimore N atom generation.

Figure 4-29 shows the results for ϕ=0.9. Again, there is essentially no effect on NO as expected.

4.3.3.4 Secondary Stage Burnout and Dilution

The function of the second stage combustor is to complete the energy release and dilute the combustion products to a suitable turbine inlet temperature. The turbine inlet temperature for the adiabatic gas turbine combustor is 2800°F.

The challenge for the second stage design is to minimize the production of thermal NO associated with finite rate mixing coincident with the minimization of the conversion of those nitrogen specie leaving the first stage to NO. A secondary stage following a nonoptimum primary operating at ϕ=2.0 with high HCN, NH_3, and NO is first examined to illustrate the essential features of the secondary combustor design problem. The optimum configuration with a primary zone operating at ϕ=1.33 is then addressed.

Figure 4-30 shows the MKAP analog schematic for a ϕ=2.0 nonoptimum primary stage with two possible secondary stage configurations. The upper schematic shows a combustor with secondary air addition distributed axially along the combustor. The distribution of equivalence ratio is shown below the figure under the assumption of rapid fuel/air mixing upon air admission. Note that

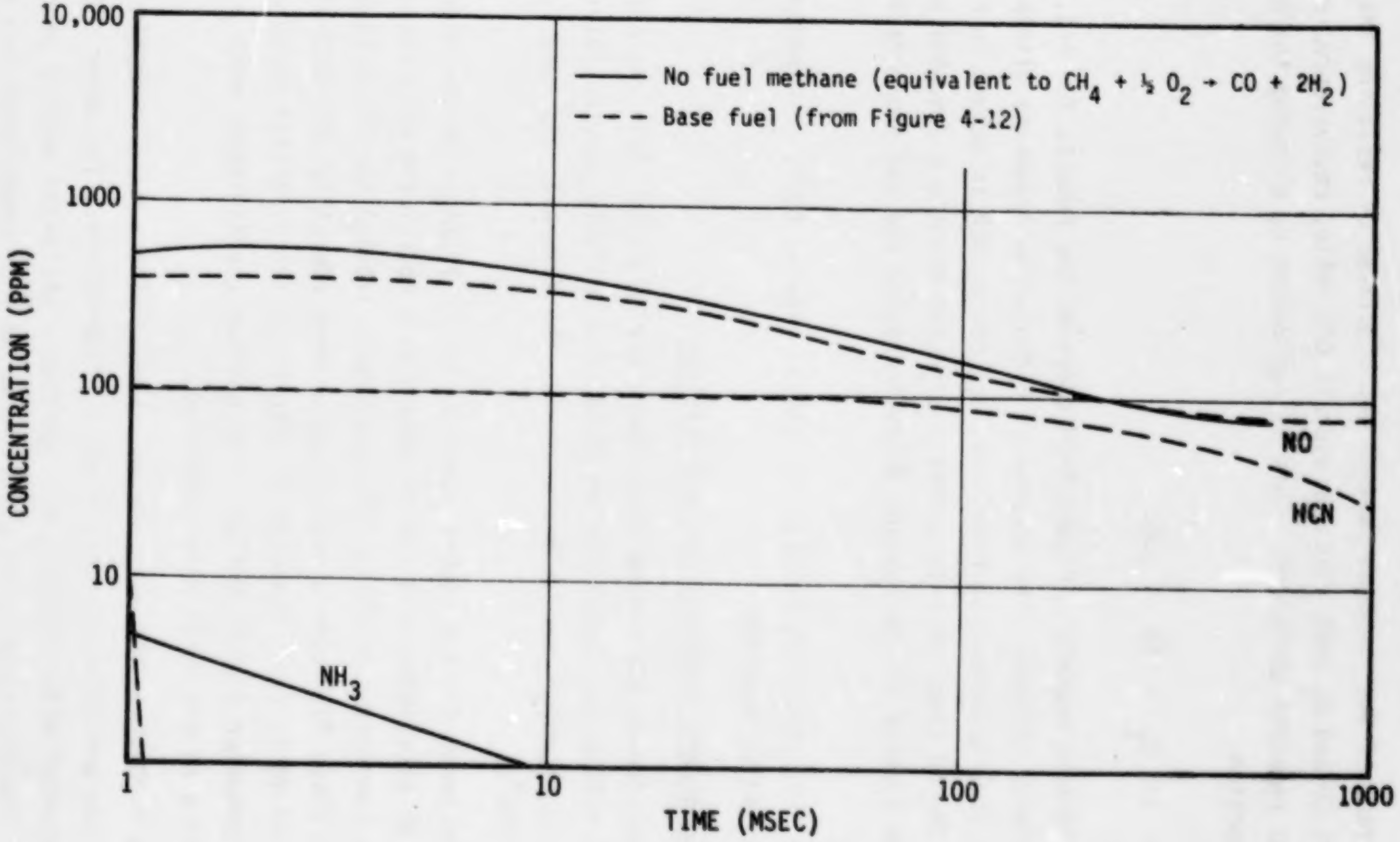


Figure 4-28. Nitrogen Species from Premixed Rich Combustion — Adiabatic Gas Turbine Combustor — Effect of Fuel Methane Content

NOTE: $\phi = 1.33$; $T_{outlet} = 3475^{o}F$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; $p = 10$ atm; $(NH_3)_0 = 2005$ ppm (4000 ppm in fuel); LOG/LOG Coordinates

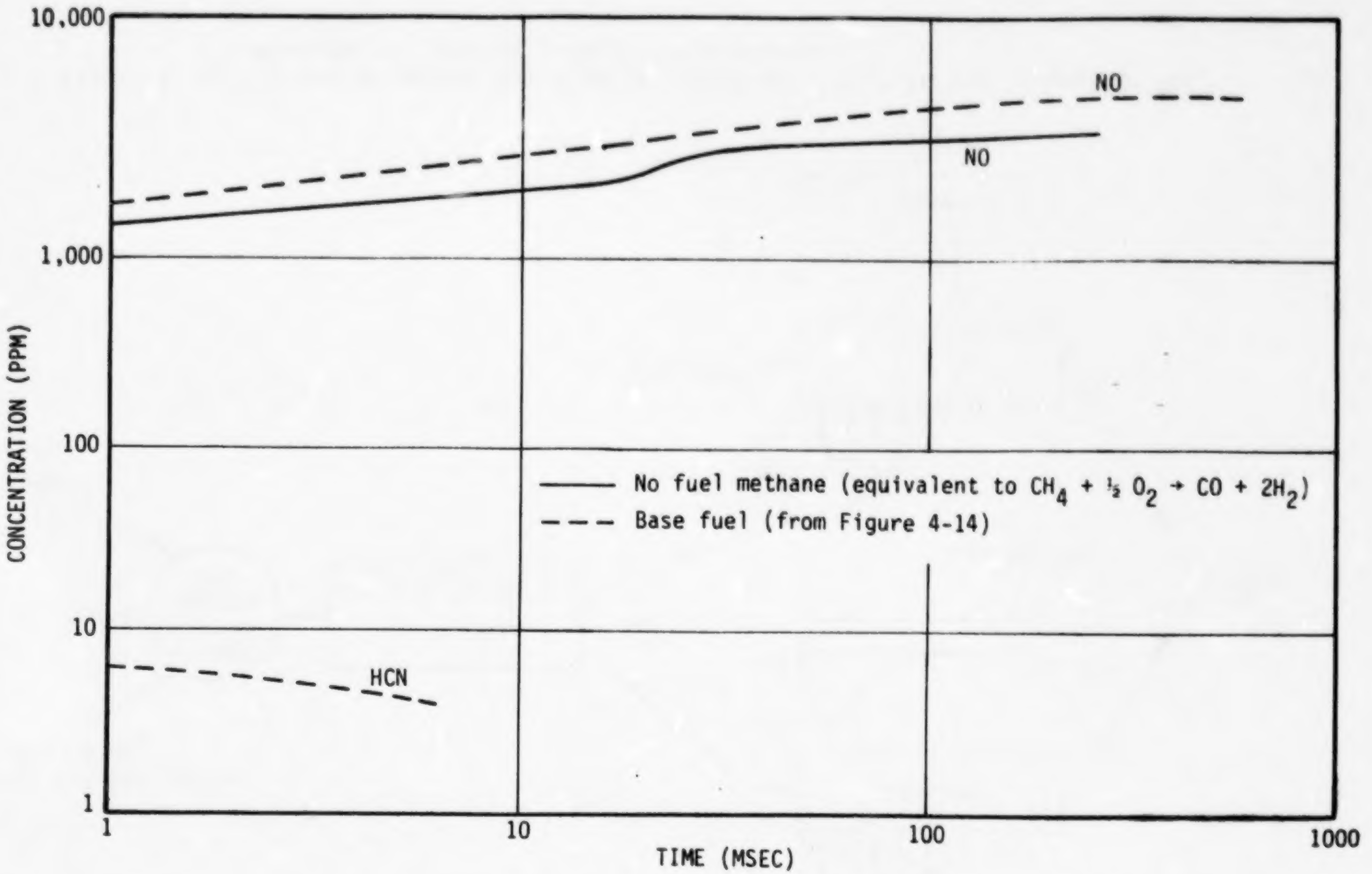


Figure 4-29. Nitrogen Species from Premixed Lean Combustion — Adiabatic Gas Turbine Combustor — Effect of Fuel Methane Content

NOTE: $\phi = 0.9$; $T_{outlet} = 3600^{o}F$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1$ msec; $(NH_3)_0 = 1706$ ppm (4000 ppm in fuel); p = 10 atm; LOG/LOG coordinates

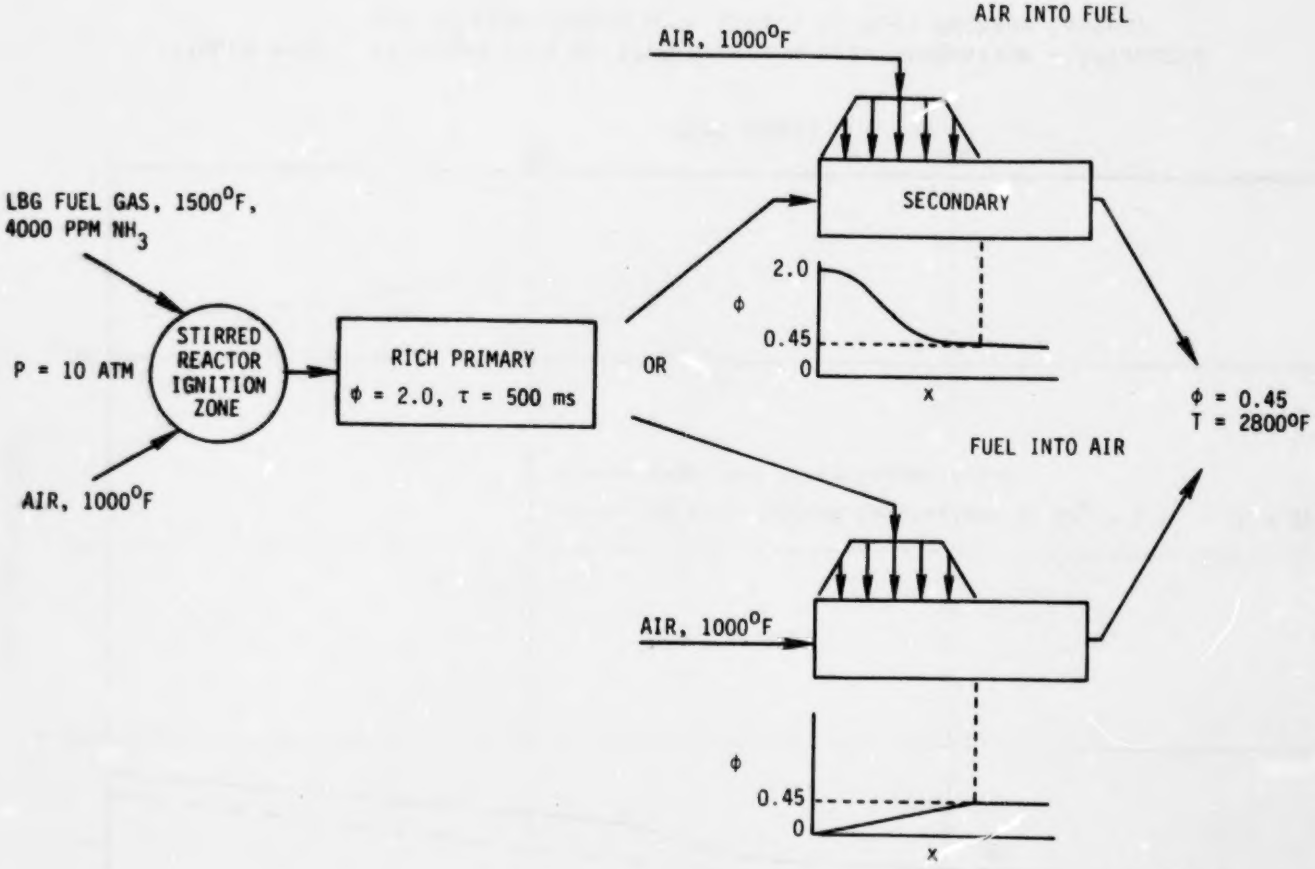
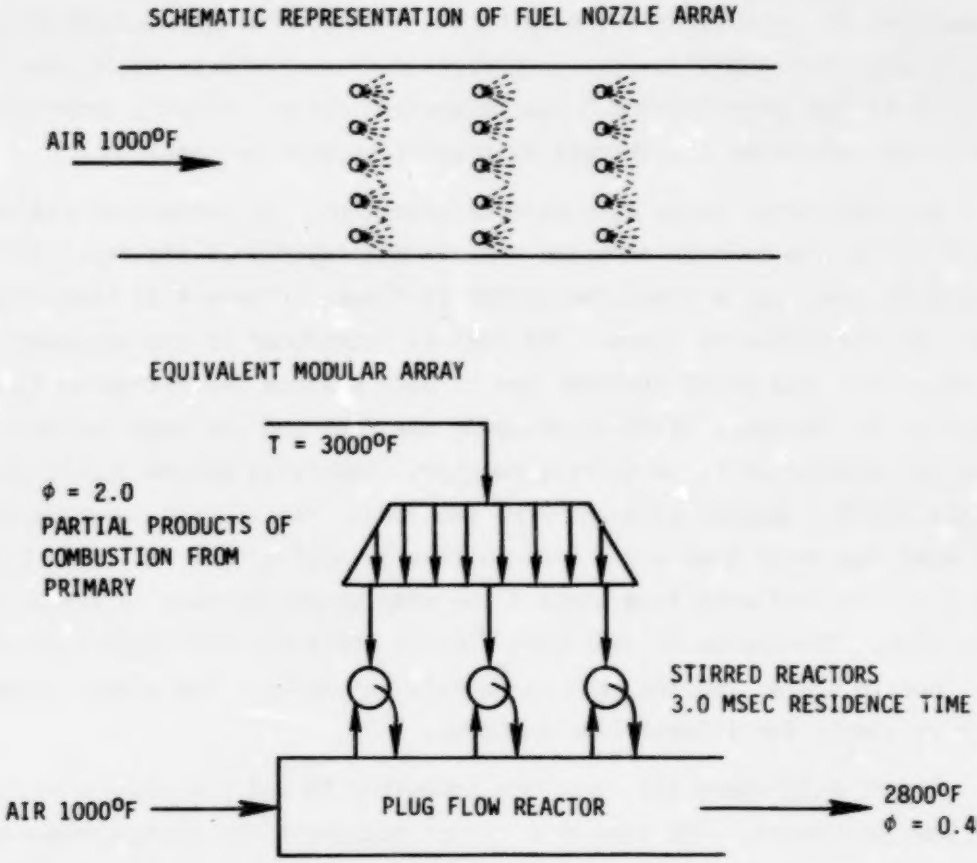

AIR INTO FUEL
AIR, 1000°F
SECONDARY
LBG FUEL GAS, 1500°F, 4000 PPM NH$_3$
2.0
ϕ
0.45
0
x
STIRRED REACTOR IGNITION ZONE
P = 10 ATM
RICH PRIMARY
ϕ = 2.0, τ = 500 ms
OR
ϕ = 0.45
T = 2800°F
FUEL INTO AIR
AIR, 1000°F
AIR, 1000°F
ϕ
0.45
0
x

Figure 4-30. Staged Adiabatic Gas Turbine Combustor – MKAP Analog Schematics for Alternative Secondary Stage Arrangements

it passes from an initial rich value of 2.0 through stoichiometric conditions to a final lean condition of 0.45. If the time constant of this delayed mixing process is substantial, considerable thermal NO will be produced during the temperature excursion near $\Phi=1$. To emphasize this behavior a mixing time constant of 50 msec was chosen for the computations. The lower schematic represents the opposite mixing limit in which the fuel is added to the secondary combustion air in a distributed fashion. Again, under the assumption of rapid mixing upon fuel admission the distribution of equivalence ratio goes from zero to 0.45 without experiencing a stoichiometric state. Clearly under these idealized conditions the thermal NO production will be small.

Two additional cases also deserve attention. Instantaneous mixing in which all of the primary products and air mix rapidly at the inlet to the secondary zone, and a simulated diffusion flame. Figure 4-31 shows the MKAP model of the diffusion flame. The fuel is introduced to the secondary air at three discrete axial stations and at each station the diffusion flame behavior is simulated by first bringing the fuel and air into contact in a parallel cluster of three stirred reactors (indicated schematically as a single stirred reactor at each entry station). The stirred reactors have a 3.0 msec residence time and a distribution of equivalence ratios of 0.9, 1.0 and 1.1. The effluent from these flame simulations is then returned to the main flow. The choice of residence time is arbitrary and implicitly reflects fuel nozzle scale, spacing, and turbulence intensity. The 3 msec value used here is simply for illustrative purposes.

Figure 4-32 shows the secondary combustor NO and temperature distribution for the four cases. The long dash curves represent the instantaneously mixed situation. In that case NO rises rapidly in the first few msec as the primary zone NO precursors are converted to NO. The NO level is lower than the primary exit only due to distribution. Following this "prompt" secondary conversion the NO increases very slowly due to thermal fixation since the temperature does not exceed 2800^{o}F. The solid curves in Figure 4-32 correspond to the upper schematic of Figure 4-30. A temperature excursion to 3700^{o}F occurs and the NO level goes over 1000 ppm before decreasing back to 850 ppm by final dilution Following this there is a gradual rise in NO due to thermal fixation.


SCHEMATIC REPRESENTATION OF FUEL NOZZLE ARRAY

EQUIVALENT MODULAR ARRAY

AIR 1000°F
T = 3000°F
Φ = 2.0
PARTIAL PRODUCTS OF COMBUSTION FROM PRIMARY
STIRRED REACTORS
3.0 MSEC RESIDENCE TIME
AIR 1000°F
PLUG FLOW REACTOR
2800°F
Φ = 0.45

Figure 4-31. Staged Adiabatic Gas Turbine Combustor — MKAP Analog Schematic for Simulated Diffusion Flame

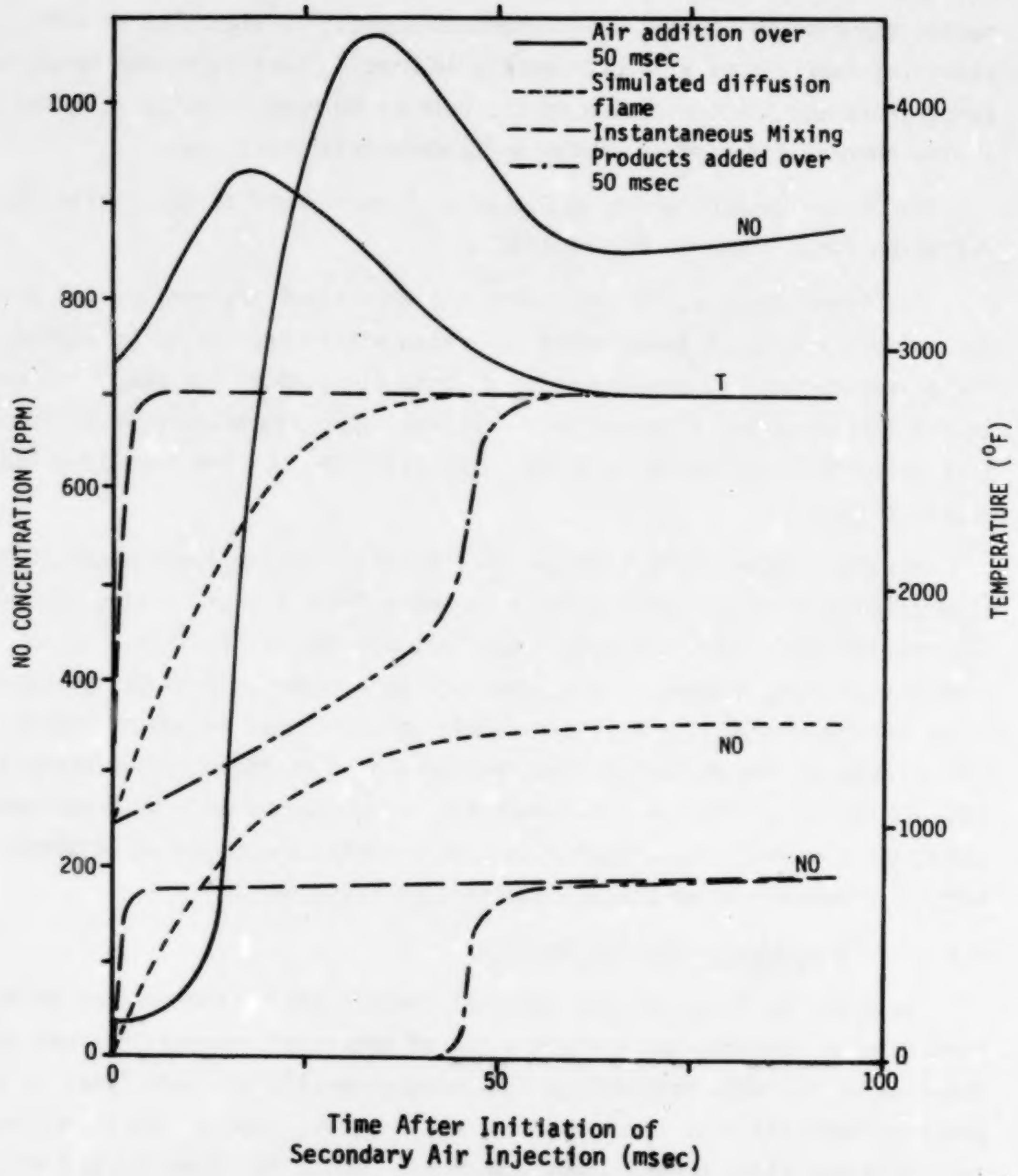


Figure 4-32. NO Concentration and Temperature for Alternative Secondary Stage Configurations — Adiabatic Gas Turbine Combustor

NOTE: Primary zone exit conditions from Figure 4-12. See Figure 4-30 for schematic.

The dot-dash curves in Figure 4-32 correspond to the lower schematic of Figure 4-30. Since fuel is added to the secondary air over a 50 msec period the mixture increases in temperature until autoignition of the remaining fuel occurs at approximately 40 msec. There is no overshoot in temperature and the conversion of the primary NO precursors is followed by a slow thermal fixation as in the instantaneously mixed case.

The short dashed curves in Figure 4-32 correspond to the finite rate diffusion flame shown in Figure 4-31.

The temperature curve represents the mean axial temperature and does not reflect the local temperature excursion within the diffusion flames. These temperature and stoichiometry distributions about the mean give rise to the increased NO as indicated. The peak flame temperature predicted by this was 3700^{o}F and produced an NO level twice that of the idealized rapid mixing case.

Finally, Figure 4-33 provides an indication of the lower bound NO emission attainable if an optimum ϕ=1.33 primary feeds a rapid mixing secondary. The results imply that NO levels under 100 ppm may be feasible. It is probably prudent, however, to assume that even under optimum design conditions finite rate mixing will contribute an additional 80 ppm of thermal NO (50 percent of the diffusion flame NO calculated in the previous example). Thus NO levels of 150 ppm can reasonably be expected from a well-designed LBG-COGAS system firing a fuel with high ammonia content in an adiabatic gas turbine combustor at an overall equivalence ratio ϕ=0.45.

4.4 Supercharged Boiler Results

In order to establish the chemical constraints on the control of NO_x formation in supercharged boilers a set of numerical computations was undertaken using the MKAP methodology following generally the same lines as the previous adiabatic gas turbine combustor analysis. Again, the objective was to derive estimates of the lower achievable limits for supercharged boiler NO_x emission as dictated by chemical considerations by exploring the dependence of NO_x emissions on specific design features.

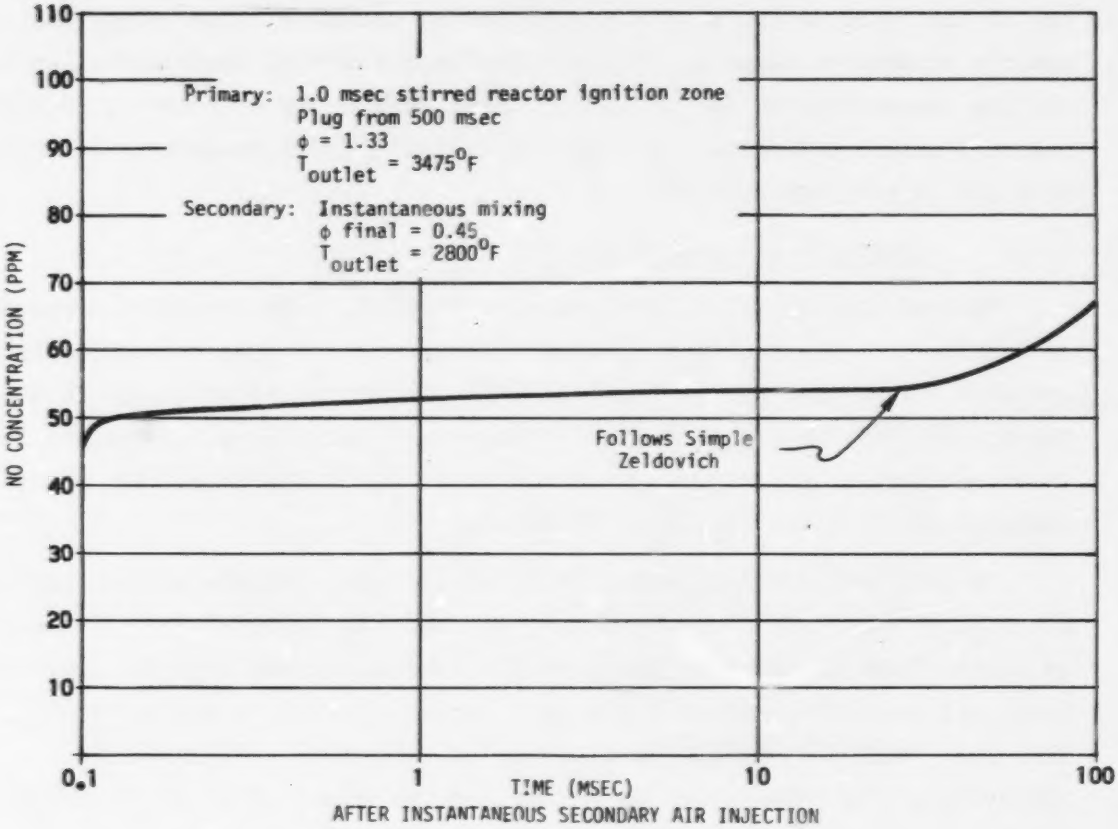


Figure 4-33. NO Concentration for Optimum Staged Adiabatic Gas Turbine Combustor

As outlined in Section 4.2, the baseline supercharged boiler system is a low excess air (5 percent) supercharged boiler firing a low temperature (150°F) fuel gas typical of the product from a coal-fired LBG gasifier with intercooling and low temperature gas cleanup. The gas composition is identical to that used in the adiabatic gas turbine combustor study except that the ammonia content is taken as 500 ppm to reflect a partial ammonia cleanup in the low temperature sulfur removal process. The boiler operates at 10 atmospheres pressure and feeds a gas turbine at 2000°F inlet temperature. Combustion air is supplied at 600°F.

4.4.1 General Flame Characteristics

Much of the general information regarding LBG flame chemistry presented in Section 4.3 is directly applicable to combustion in supercharged boilers and will not be repeated in this section. The principal difference in the two systems lies in the lower fuel nitrogen and lower flame temperature for the supercharged boiler fuel and in the nonadiabatic low excess air secondary stage combustor associated with the boiler.

Figures 4-34 and 4-35 shows the adiabatic flame temperature and equilibrium NO as functions of equivalence ratio and fuel temperature. The maximum adiabatic flame temperature 3160°F is 500°F below the gas turbine case. At 5 percent excess air the adiabatic equilibrium NO level is approximately 1000 ppm. Note how sharply the equilibrium values fall off as $\phi=1$ is approached. The peak values are located on the lean side at approximately $\phi=0.8$.

4.4.2 Premixed Lean Combustion

Figure 4-36 presents the results for a premixed lean combustor operating at 5 percent excess air. It provides an "uncontrolled" estimate of NO emission levels against which to measure the success of the staged combustion system discussed in the next section.

A 1.0 msec stirred reactor provides ignition and "prompt" conversion of essentially all of the fuel nitrogen to NO. The stirred reactor is followed by a plug flow heat exchange section. The heat transfer distribution is shown

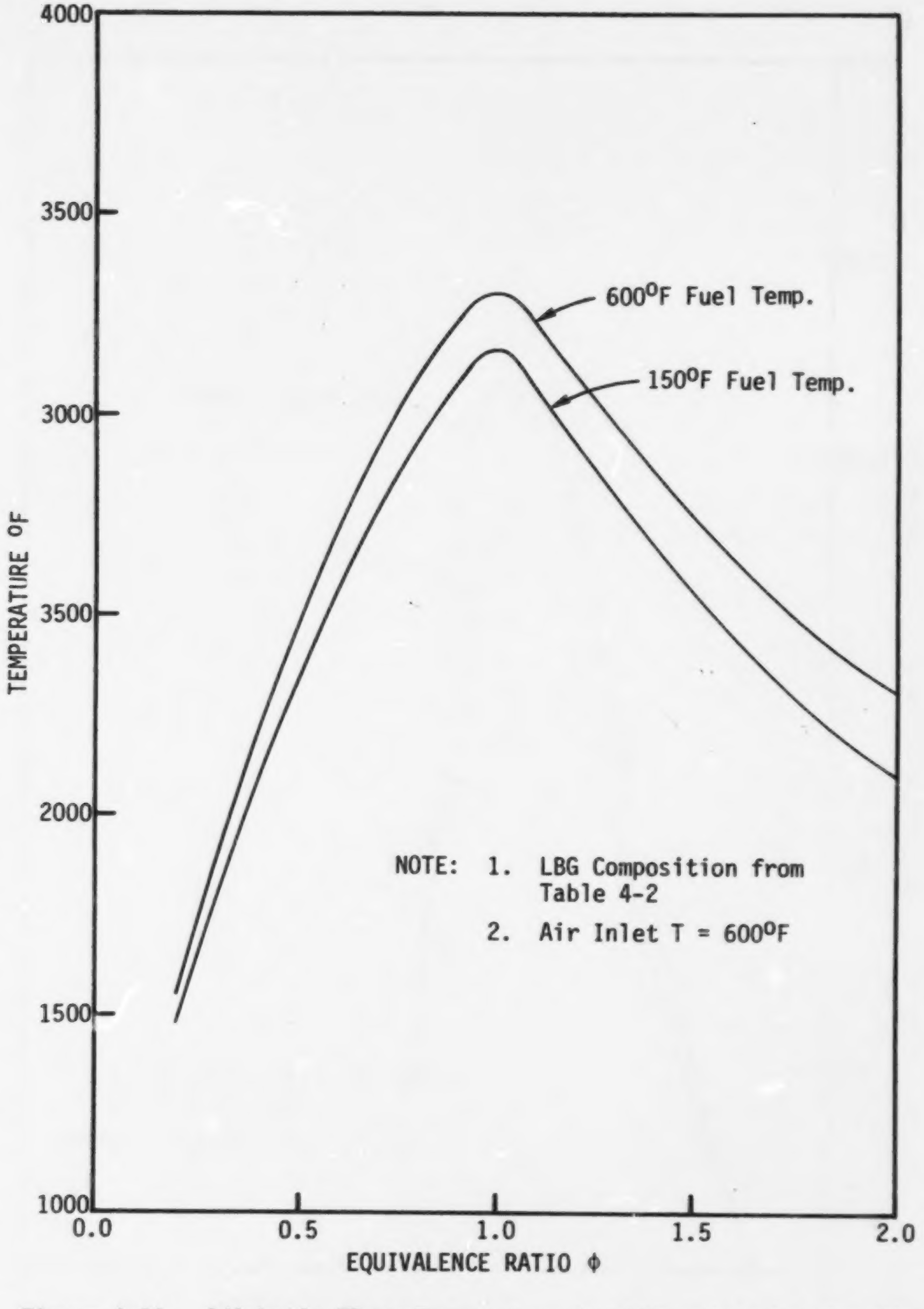


Figure 4-34. Adiabatic Flame Temperature for LBG and Combustion Air for Supercharged Boiler

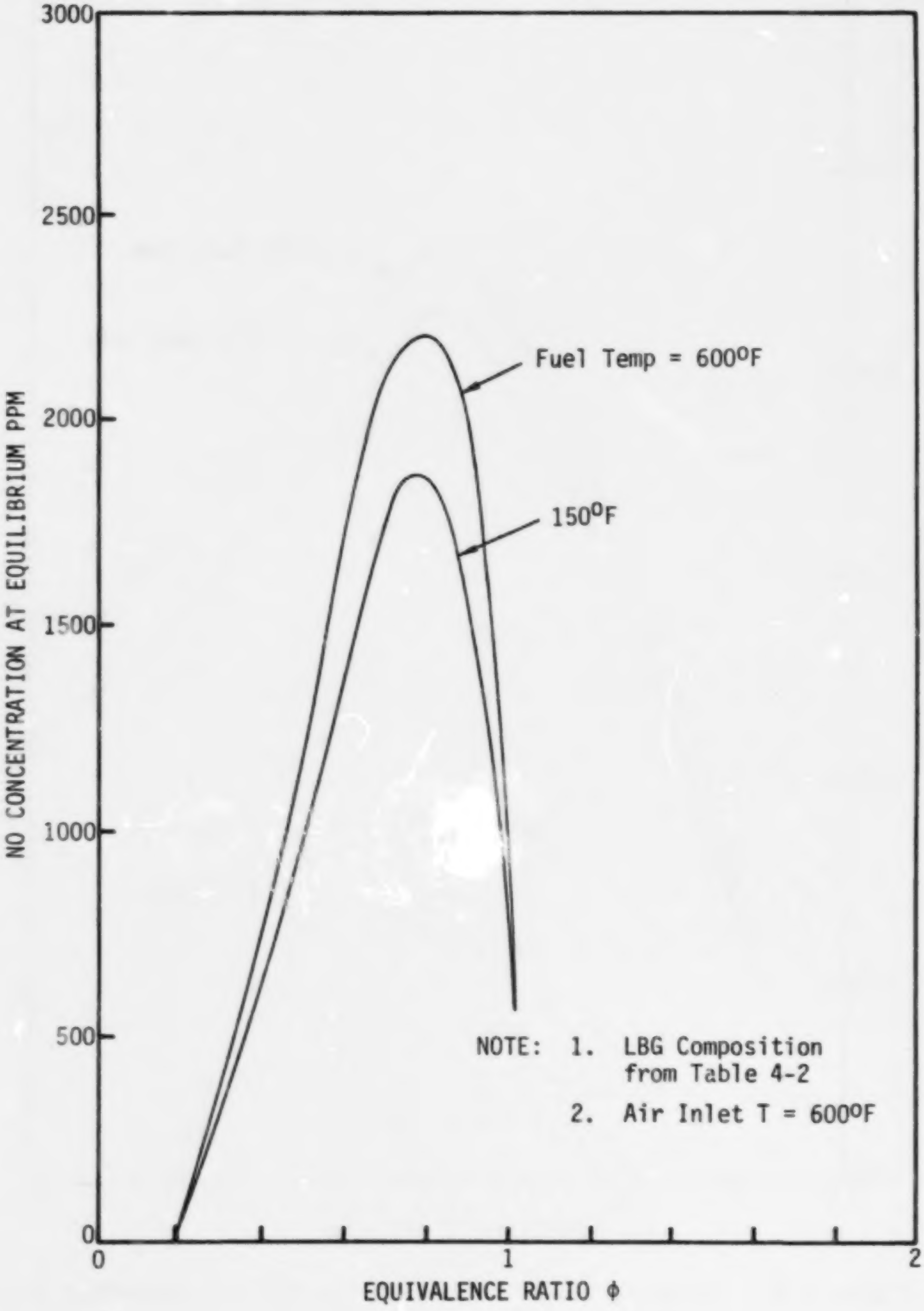


Figure 4-35. Equilibrium NO Concentrations - Supercharged Boiler

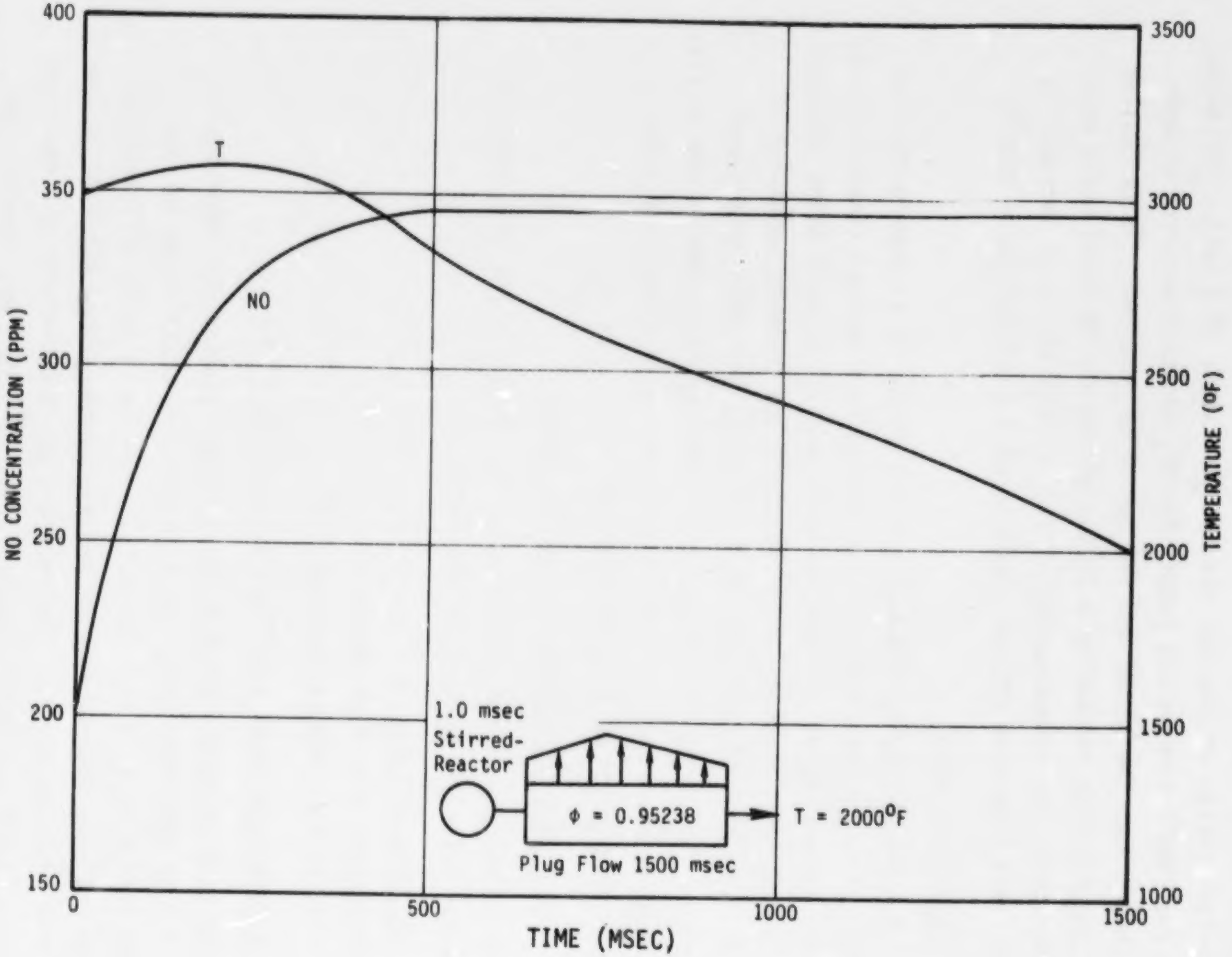


Figure 4-36. NO Concentration and Temperature for Premixed Lean Combustion — Supercharged Boiler

NOTE: 5% excess air; $(NH_3)_0$ = 500 ppm in fuel; Heat removal as shown above in Figure 4-36 and has a 2:1 peak-to-minimum ratio with the peak occurring at the midpoint of the boiler. For the purposes of this computation an arbitrarily long residence time was assumed (in excess of 1 sec). For these conditions the $2800^{\circ}F$ temperature cutoff for NO_x kinetics occurred at one-third the length down the boiler and 345 ppm of NO resulted. If the boiler residence time had been reduced by a factor of two the NO level would have been 330 indicating the insensitivity of the calculation to an increase in overall residence time once the gas temperature has dropped below $2800^{\circ}F$.

4.4.3 Staged Combustion

The objective of staging the supercharged boiler is to reduce the fuel nitrogen conversion to well below 200 ppm (based on 5 percent excess air) and to reduce the thermal NO in the heat exchange section to well below 150 ppm using the same control strategy as the adiabatic gas turbine combustor in Section 4.3. Figure 4-37 shows the MKAP schematic for the staged supercharged boiler. The additional degree of freedom present here is the ability to simultaneously stage the secondary stage heat release and heat transfer to minimize long periods at high temperature.

4.4.3.1 Fuel-Rich Primary Stage — Baseline Case

The following discussion addresses the NO_x kinetics for this baseline reactor as the following parameters are varied:

- Equivalence ratio, ϕ
- Adiabatic plug flow residence time, τ
- Initial fuel ammonia content, $(NH_3)_0$

Equivalence Ratio and Plug Flow Residence Time

Figures 4-38 through 4-41 show the nitrogen species and temperature histories for an adiabatic plug flow rich primary operating at various equivalence ratios (1.5, 1.4, 1.33, 1.15). The ignition in all cases was provided by a 2 msec stirred reactor and all of the prompt behavior is confined to this ignition device. The fuel and air temperatures are the baseline values of $150^{\circ}F$ and $600^{\circ}F$, respectively. The fuel NH_3 level is the baseline value of 500 ppm.

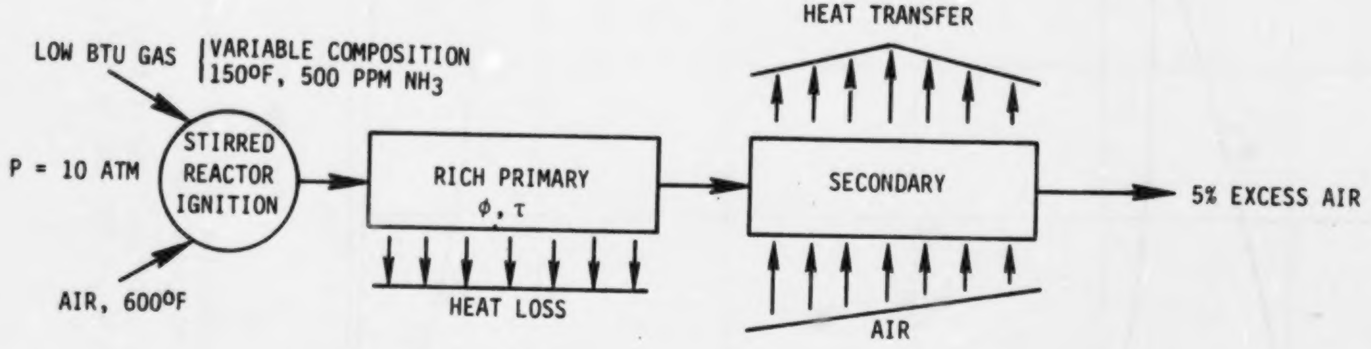

HEAT TRANSFER
LOW BTU GAS
VARIABLE COMPOSITION
150°F, 500 PPM NH3
STIRRED REACTOR IGNITION
P = 10 ATM
AIR, 600°F
RICH PRIMARY
φ, τ
HEAT LOSS
SECONDARY
AIR
5% EXCESS AIR

Figure 4-37. Staged Supercharged Boiler — MKAP Analog Schematic

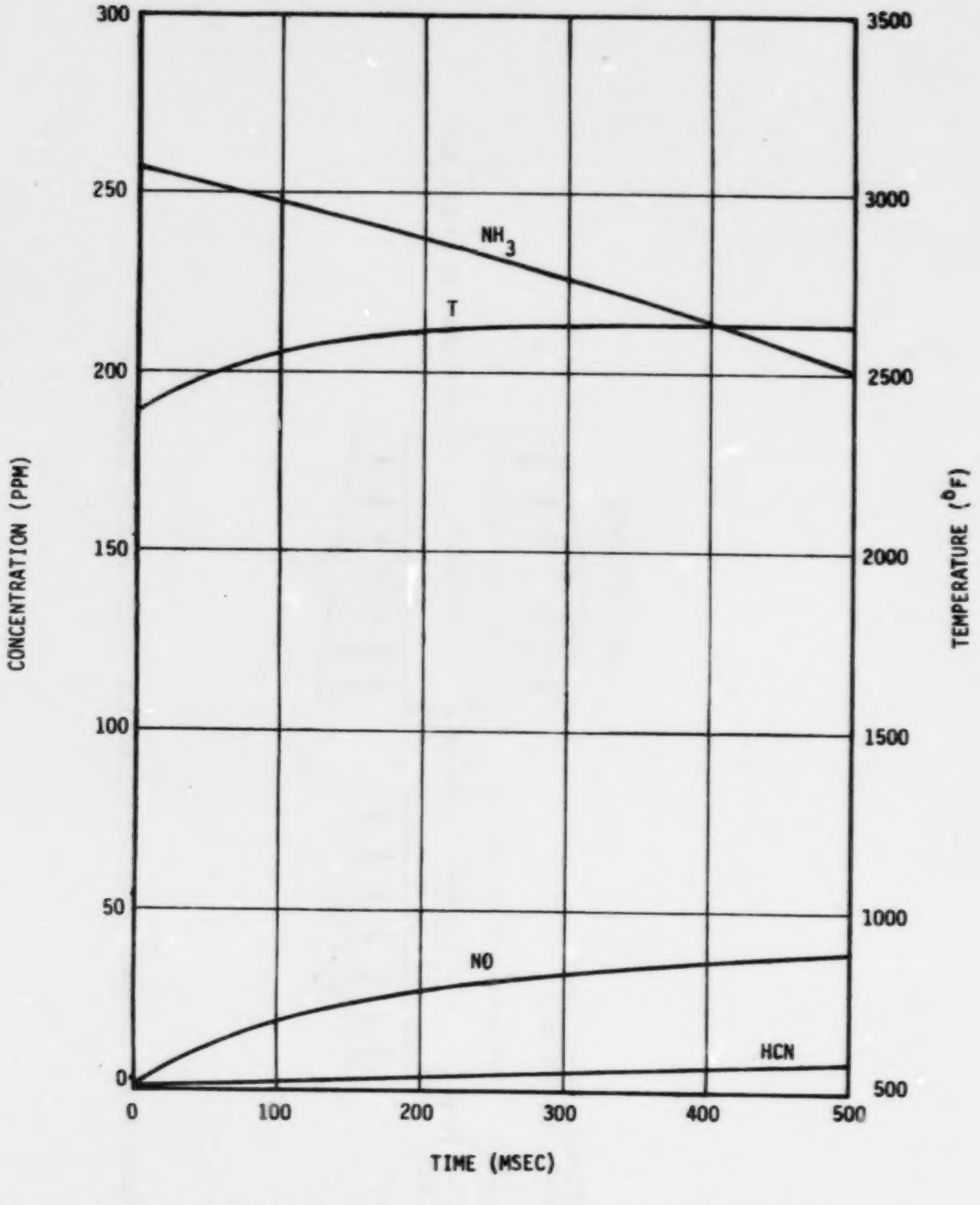


Figure 4-38. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: ϕ = 1.5; Ordinate values from stirred reactor ignition zone τ_{SR} = 1.0 msec; NH_3 = 500 ppm in fuel; No heat transfer

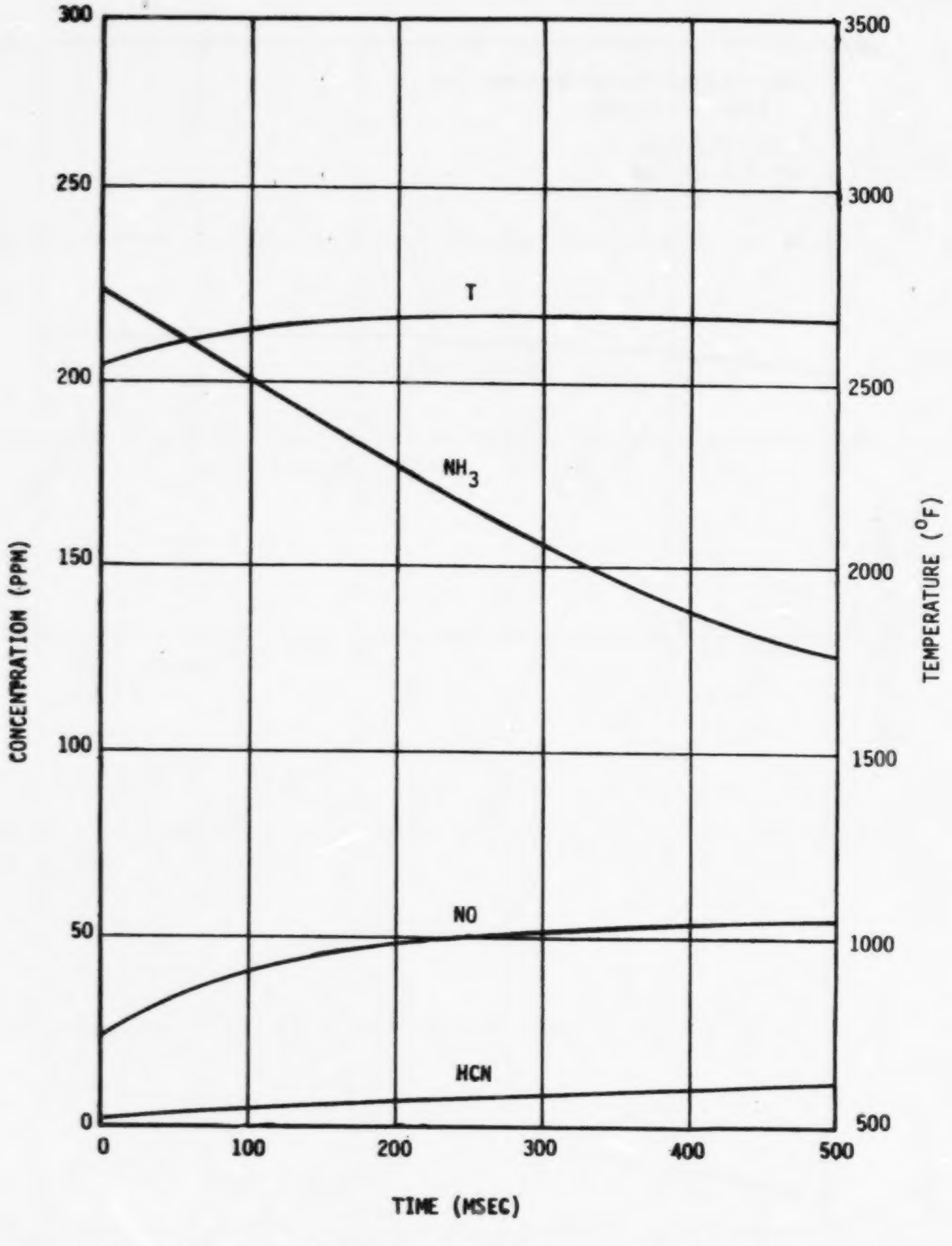


Figure 4-39. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: $\phi = 1.4$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; NH_3 = 500 ppm in fuel; No heat transfer

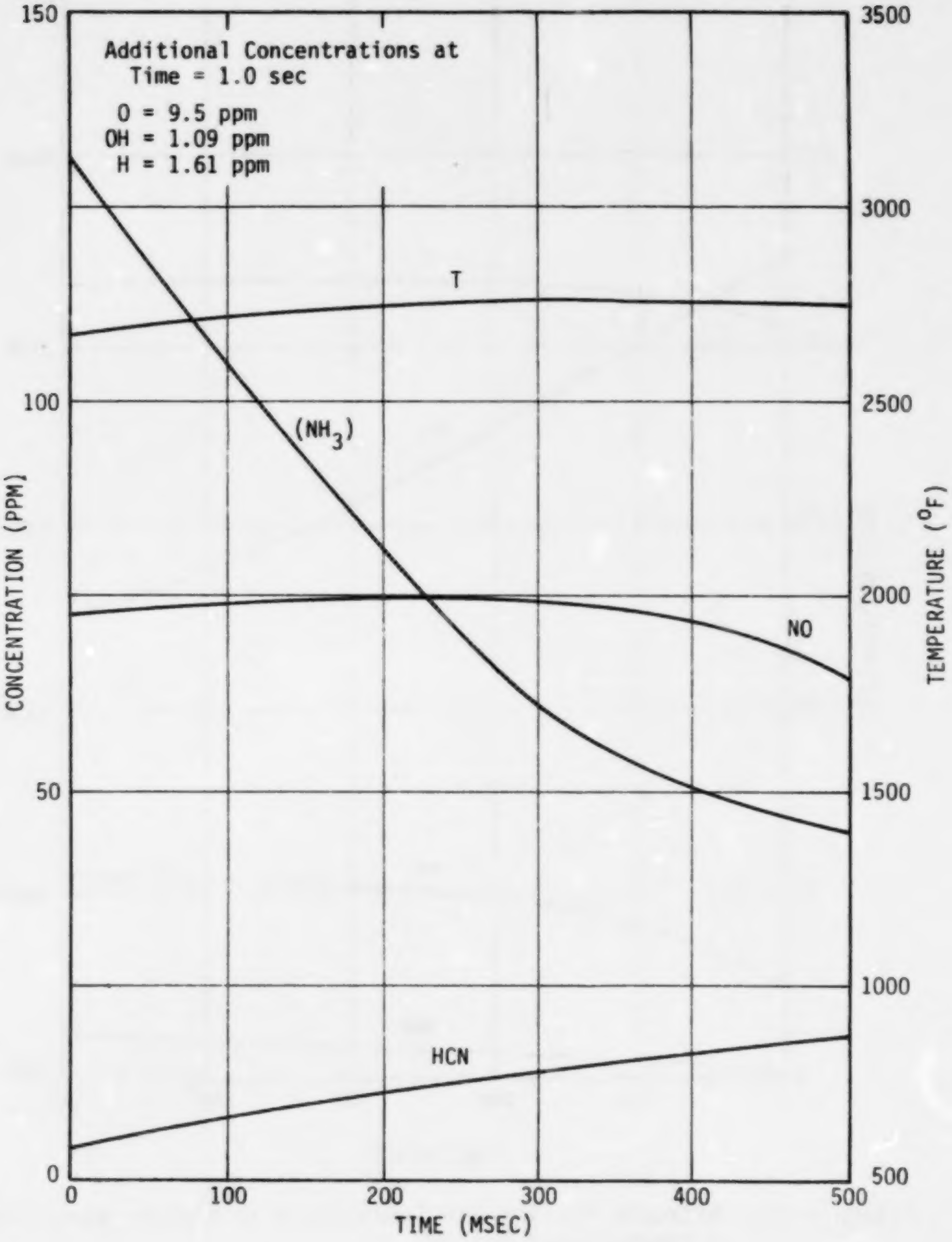


Figure 4-40. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: $\Phi = 1.33$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; $(NH_3)_0 = 263$ (500 ppm in fuel); No heat transfer

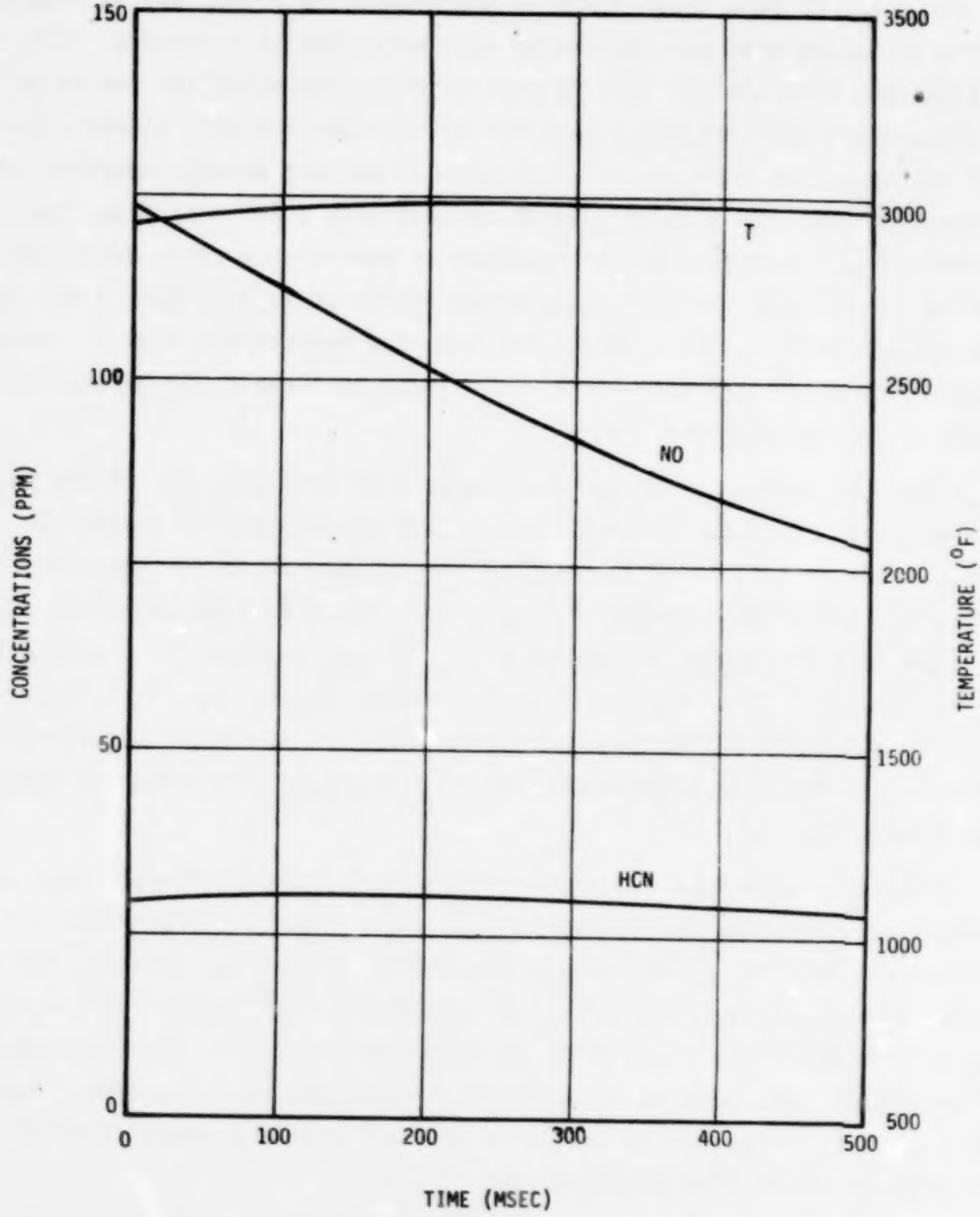


Figure 4-41. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: ϕ = 1.15; Ordinate values from stirred reactor ignition zone τ_{SR} = 1.0 msec; $(NH_3)_0$ = 243 (500 ppm in fuel); No heat transfer

For $\Phi=1.5$ (Figure 4-38) there is practically no prompt fuel-N reduction and the situation does not improve as residence time is increased. This is distinguished from the gas turbine rich primary zone situation for which the temperature and fuel ammonia concentration were considerably higher. For $\Phi=1.4$ the situation improves slightly with 15 percent prompt reduction of the NO precursor species increasing to 30 percent with a 200 msec plug flow residence time. HCN generation increases as equivalence ratio decreases becoming significant for only equivalence ratios of 1.33 (Figure 4-40) and lower (Figure 4-41). For richer conditions the hydrocarbon radical concentrations are apparently not sufficiently large to promote HCN generation at the low prevailing temperatures.

Under the leaner conditions in Figures 4-41 ($\phi=1.15$), all of the NH_3 vanishes in the 1.0 msec stirred reactor leaving substantial NO and HCN. Although this appears to be the optimum equivalence ratio for the reduction of NO precursors, the "prompt" reduction is only 36 percent and after a 200 msec plug flow residence the reduction of nitrogen species (NO precursors) is only 45 percent. This 10 percent further reduction corresponds to approximately 20 ppm corrected to 5 percent excess air. This small improvement is probably not worth the large combustor size required for a long residence time primary zone.

Finally, Figure 4-42 provides a composite picture of primary zone effectiveness as a function of equivalence ratio and time by plotting the sum of the nitrogen-bearing species normalized by the initial fuel ammonia concentration against equivalence ratio. In comparison with Figure 4-17, a similar plot for the adiabatic gas turbine combustor primary zone, the supercharged boiler primary zone reduces a smaller portion of the fuel nitrogen. Further investigation is required to determine whether this is a temperature or a fuel nitrogen concentration effect.

Initial Fuel Ammonia Content

Figures 4-43 through 4-45 are for $\Phi=1.33$ with a fuel NH_3 content of 0, 250, and 1000 ppm. The HCN distributions remain unchanged since the Fenimore mechanism is the dominant producer of HCN. In comparison with Figure 4-40,

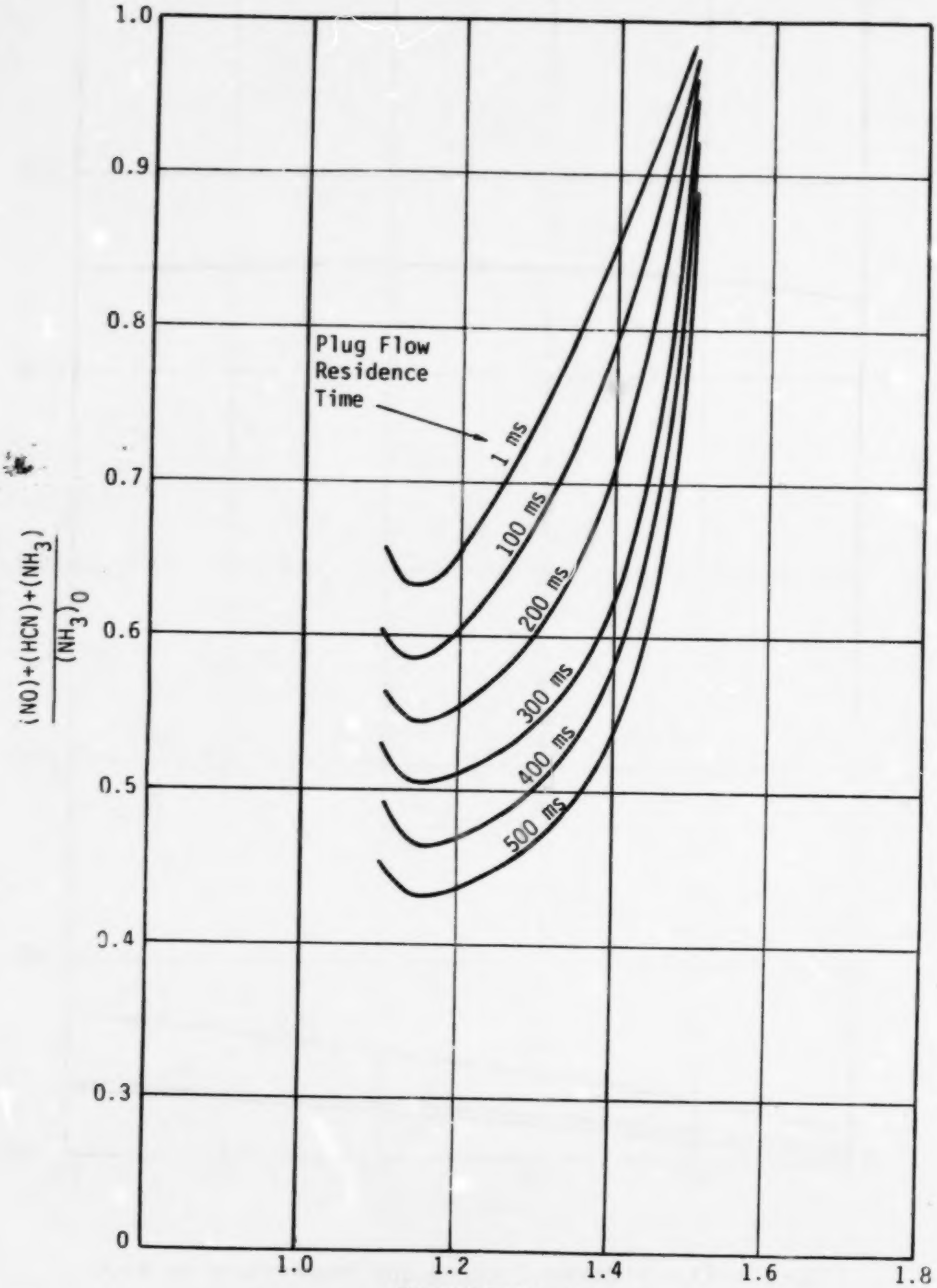


Figure 4-42. Sum of Residual Nitrogen Species from Premixed Plug Flow Primary — Supercharged Boiler

NOTE: Stirred reactor ignition zone τ_{SR} = 1.0 msec); $(NH_3)_0$ = 500 ppm in fuel

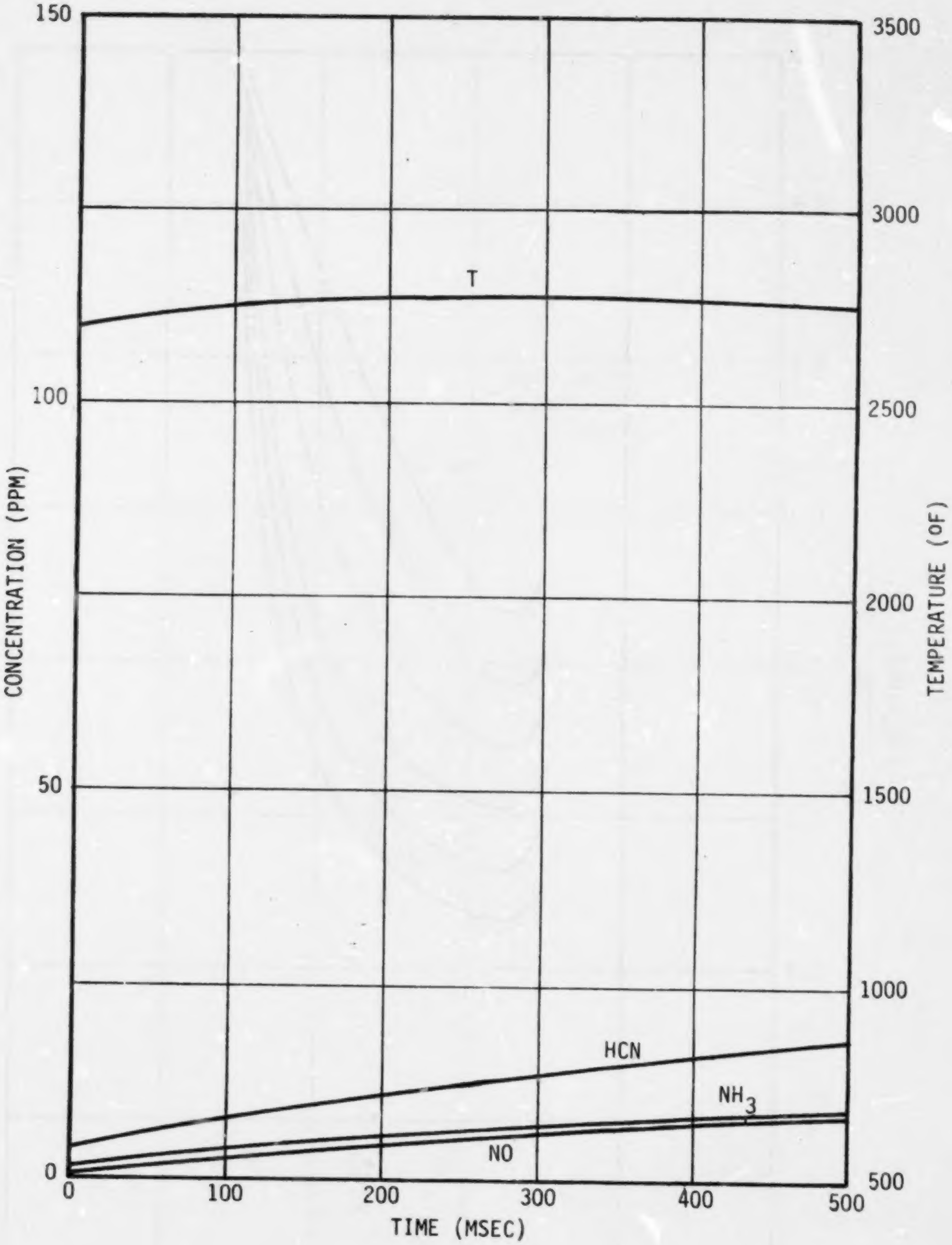


Figure 4-43. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: $\phi = 1.33$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; $(NH_3)_0 = 0$; No heat transfer

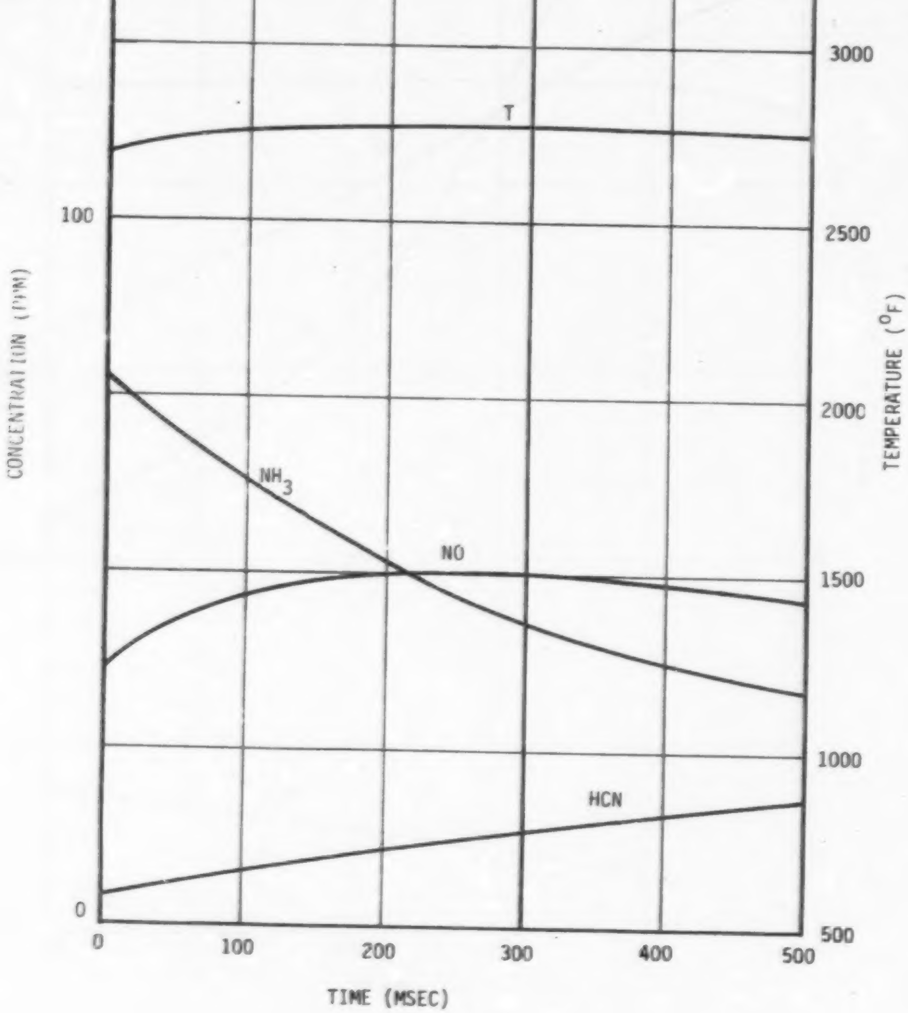


Figure 4-44. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: $\phi = 1.33$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; $(NH_3)_0 = 132$ ppm (250 ppm in fuel); No heat transfer

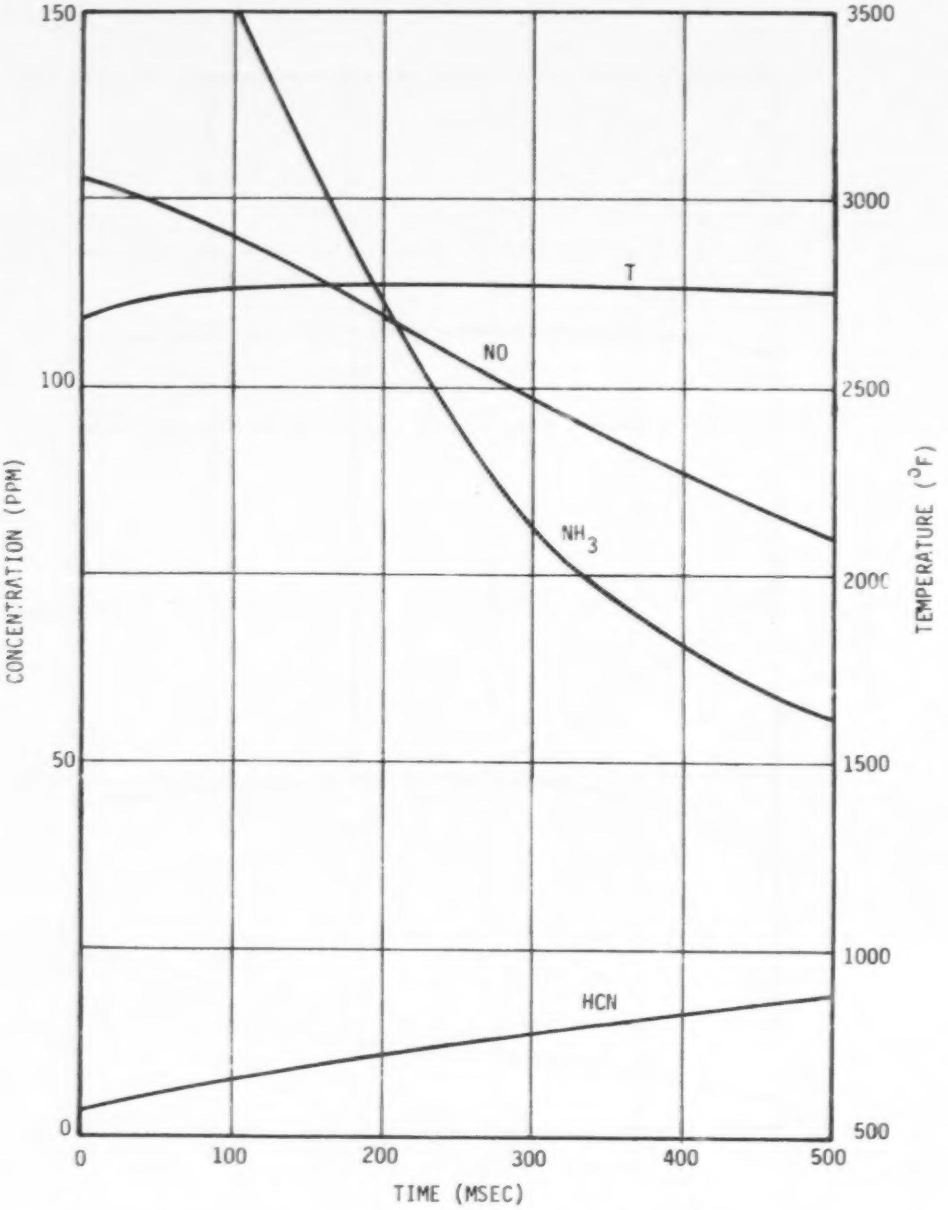


Figure 4-45. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: $\phi = 1.33$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; $(NH_3)_0 = 526$ ppm (1000 ppm in fuel); No heat transfer the baseline case with fuel NH_3 = 500 ppm, the results shown on these figures are as expected with one exception. For the case of no NH_3 in the fuel (Figure 4-43) there is a synthesis of a small amount of NH_3 (10 ppm) over 500 msec. One can speculate that this is due to N and NH atom generation through the Fenimore reactions. These in turn would combine with OH radicals to eventually form NH_3.

4.4.3.2 Deviations from Baseline Primary Reactor Specifications

Now that the factors influencing NO_x production in the baseline primary reactor have been discussed, the following additional variables will be addressed:

- Pressure
- Stirred reactor residence time
- Heat transfer from plug flow reactor
- Fuel composition - methane content

Pressure Effects

Figures 4-46 and 4-47 show the effects of reduced pressure on the ϕ=1.33 baseline case. The pressure levels are 1.0 and 0.1 atmospheres, respectively. The kinetically-limited NO levels increase with reduced pressure similar to the equilibrium NO level. The NH_3 levels are essentially zero at these lower pressures with equilibrium strongly favoring NO. The HCN concentrations also diminish as pressure is dropped.

One of the reasons for selecting reduced pressures is to provide computational data to compare with experimental HCN data from one atmosphere and lower pressure flames. In general, the experimental results have not exhibited the relatively high predicted levels of HCN for high pressure conditions. It now appears that HCN is generated only under restricted conditions of temperature, pressure, equivalence ratio, fuel composition, and degree of backmixing (e.g., stirred reactor residence time). Conditions favoring HCN generation are high temperature, high pressure, high CH_4 content, and a high degree of backmixing. Under these conditions HCN synthesis increases with increasing equivalence ratio. For example, in comparing the supercharged boiler with the

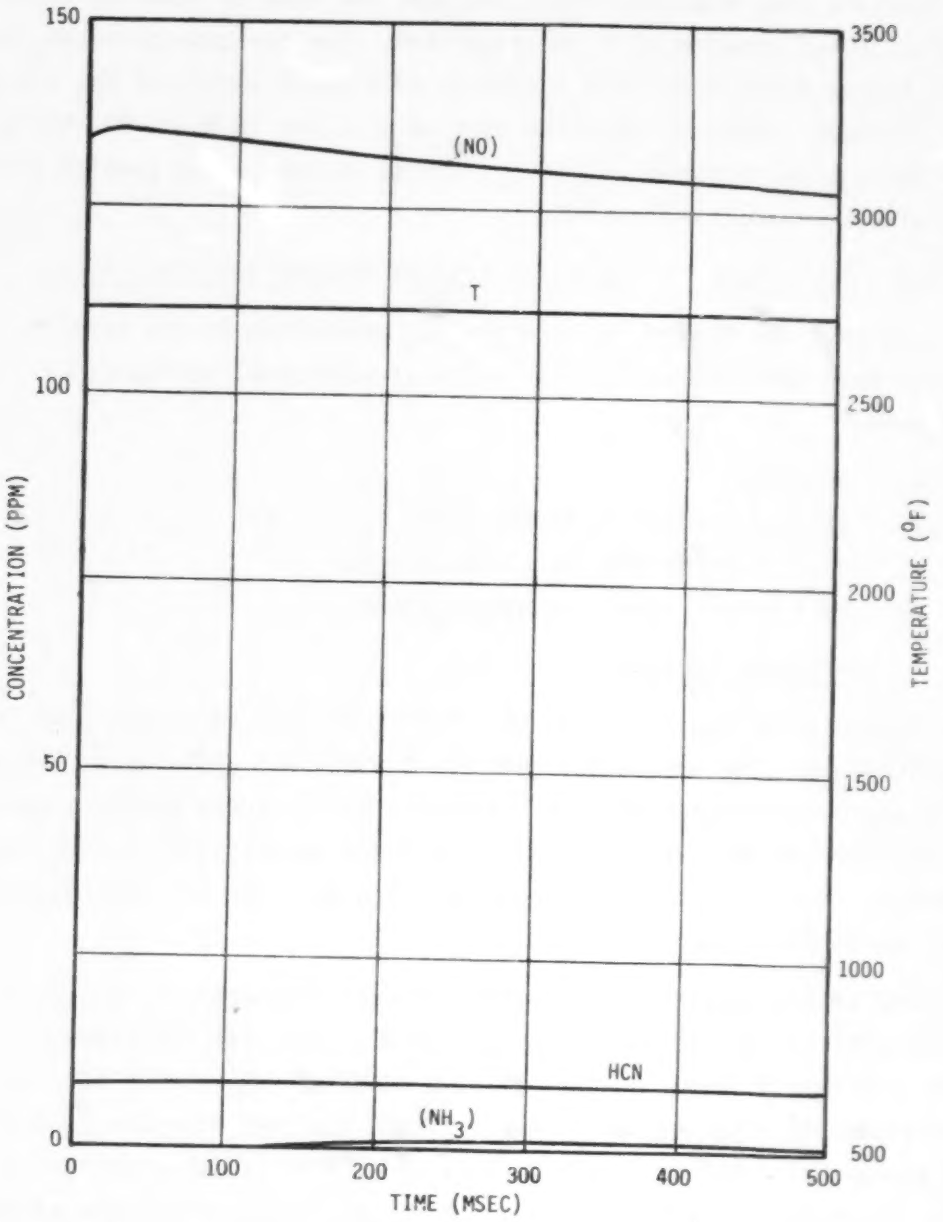


Figure 4-46. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: ϕ = 1.33; Ordinate values from stirred reactor ignition zone τ_{SR} = 1.0 msec; $(NH_3)_0$ = 263 (500 ppm in fuel); No heat transfer; Pressure = 1.0 atm

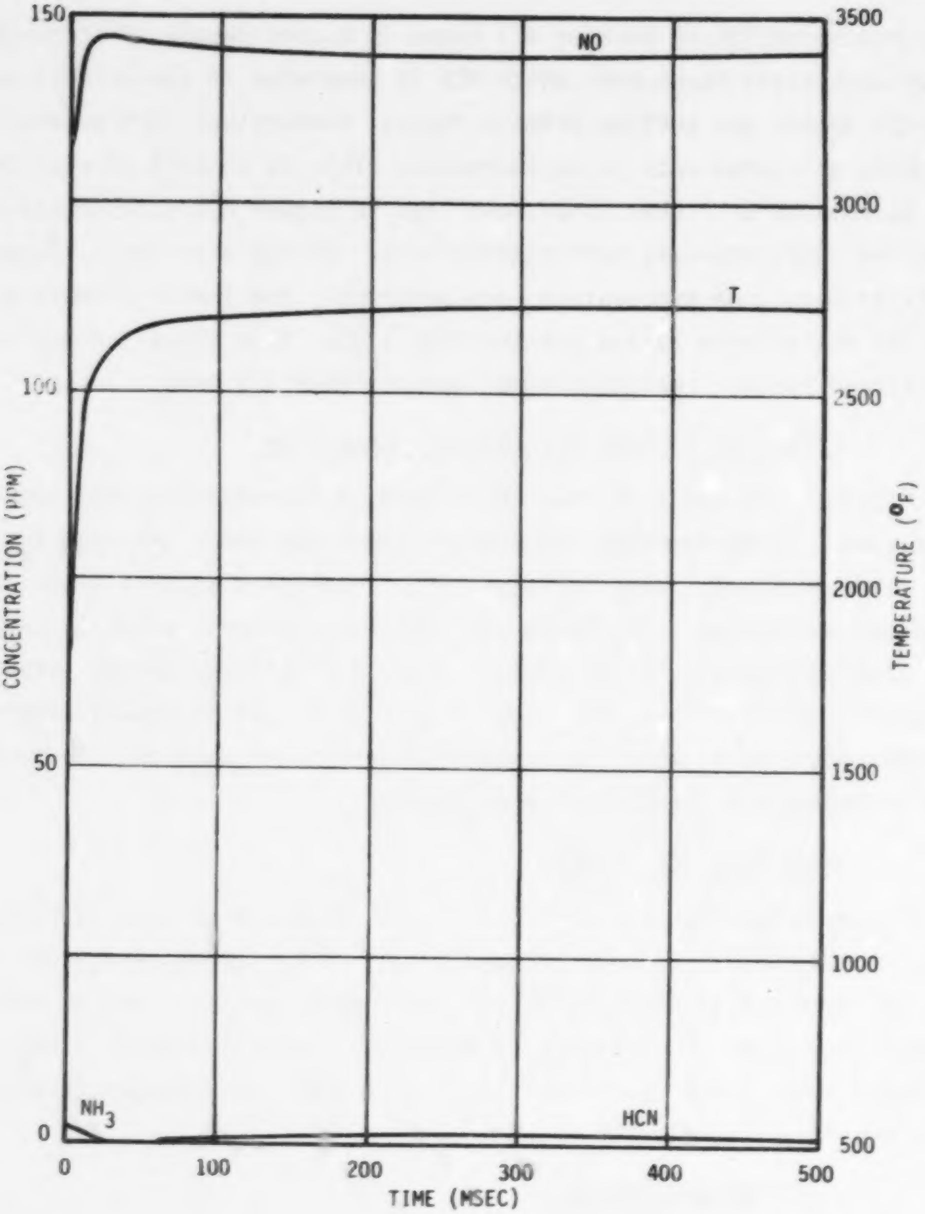


Figure 4-47. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: $\phi = 1.33$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; $(NH_3)_0 = 263$ (500 ppm in fuel); No heat transfer; Pressure = 0.1 atm gas turbine results of Section 4.3 there is a considerable difference in the equivalence ratio range over which HCN is generated in appreciable quantities. With the higher gas turbine primary reactor temperature, HCN generation increases as equivalence ratio increases. This is consistent with the notion that backmixing or richer conditions lead to higher hydrocarbon radicals provided the temperature is sufficiently high. On the other hand, supercharged boiler primary zone temperatures are apparently too low to promote HCN generation for equivalence ratios greater than 1.33. This situation may be altered for stirred reactor residence times greater than 1.0 msec.

Effect of Stirred Reactor Residence Time

Figures 4-48 and 4-49 show the effect of increased stirred reactor residence time. Large increases of HCN are indicated which are apparently due to a correspondingly large increase in hydrocarbon fragments associated with increased backmixing. NO levels also increase somewhat which is probably due to N atom generation via the Fenimore reaction followed by the extended Zeldovich reactions (N + OH). The overall effect of increased stirred reactor residence time is to make the systems appear richer with an attendant decrease in nitrogen species reduction effectiveness.

Heat Transfer Effects

Figure 4-50 shows the effect of a distributed heat loss corresponding to 200^0F for the ϕ=1.15 case (Figure 4-41). Under these conditions the heat loss has very little effect which is consistent with the results obtained in Section 4.3 for the gas turbine analysis. A small amount of NH_3 is generated under these conditions indicating that lower temperatures favor these synthesis reactions.

Fuel Methane Content

Figure 4-51 presents the ϕ=1.33 case with the methane content allowed to go instantaneously to CO and H_2. Comparison should be made with Figure 4-40. In the absence of methane the O, OH and H radical concentrations are increased by large factors as indicated on the two figures and as a consequence the prompt NH_3 reduction is much larger and the prompt reduction of NO precursors is over 70 percent. The synthesis of NH_3 could be initiated by the presence of the large H content combining with N_2 to yield N and NH.

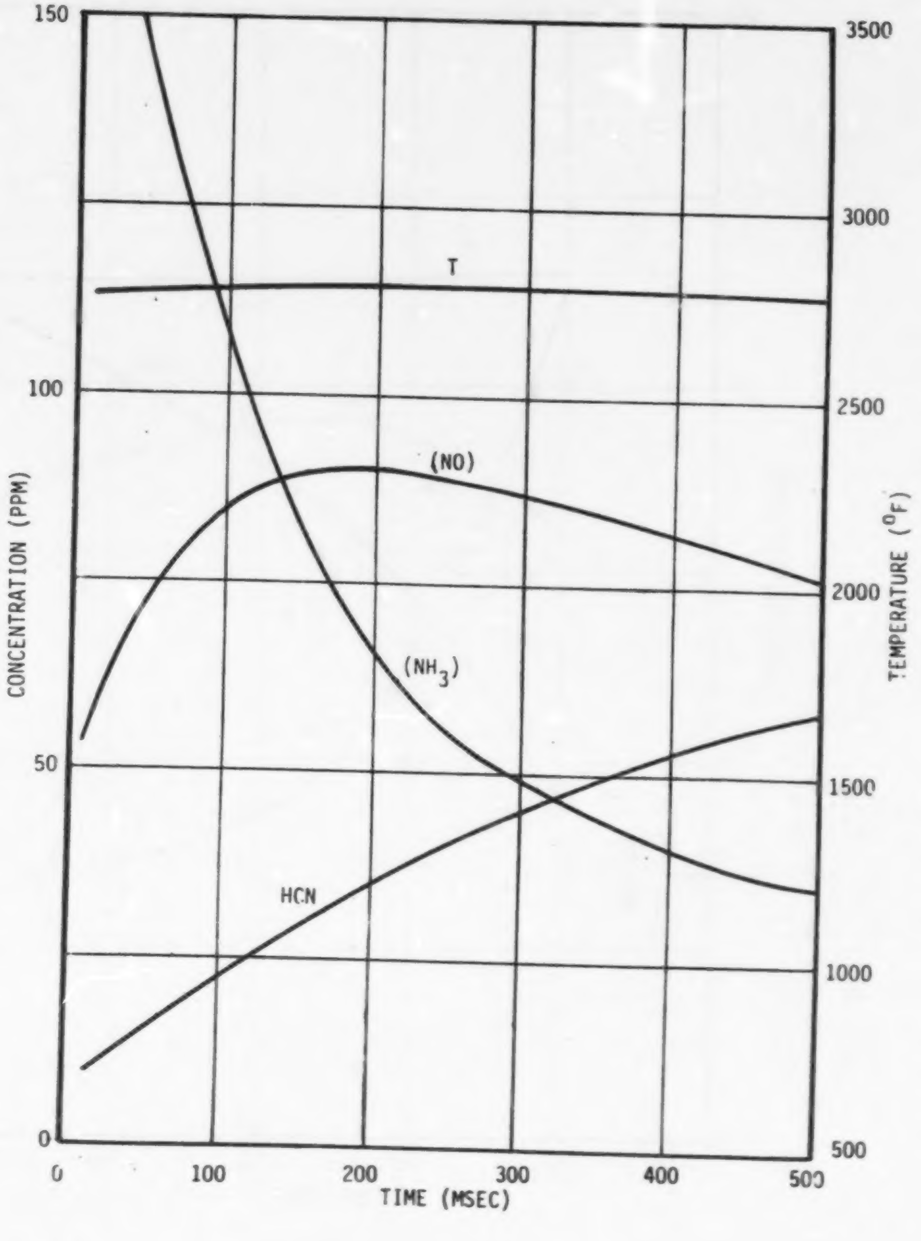


Figure 4-48. Nitrogen Species and Temperature in Rich Primary Zone – Supercharged Boiler

NOTE: $\phi = 1.33$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 10$ msec; NH_3 = 500 ppm in fuel; No heat transfer

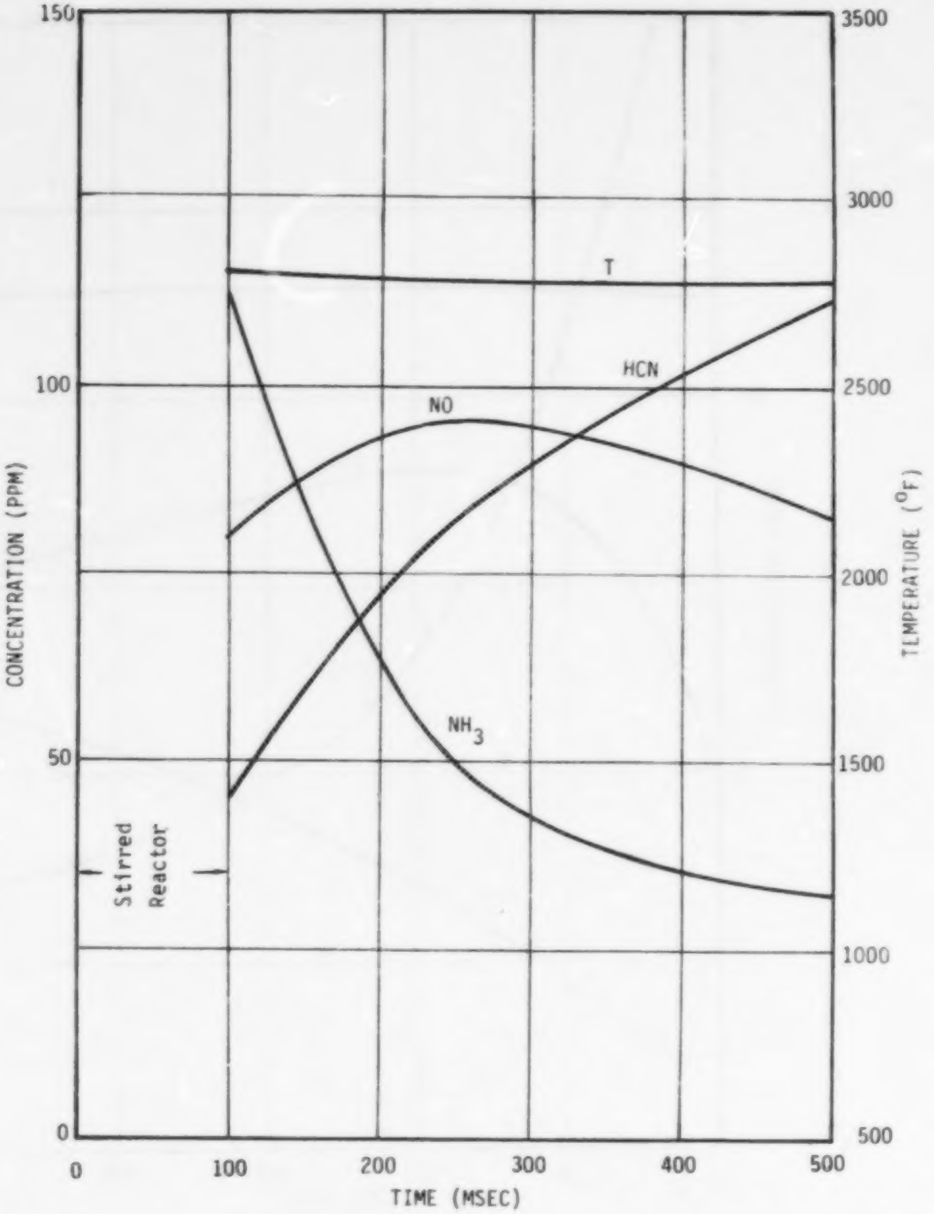


Figure 4-49. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: $\phi = 1.33$; Ordinate values from stirred reactor ignition zone τ_{SR} = 100 msec; NH_3 = 500 ppm in fuel; No heat transfer

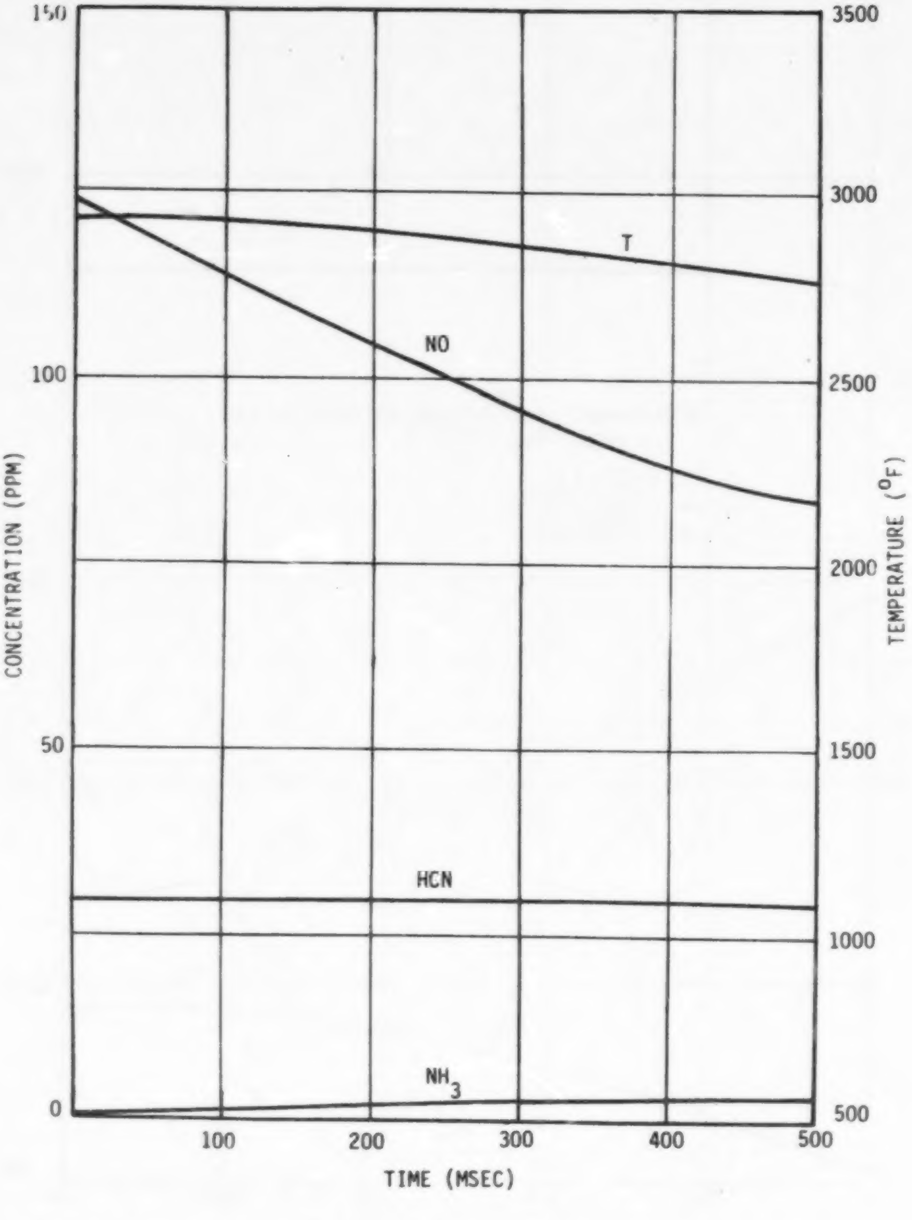
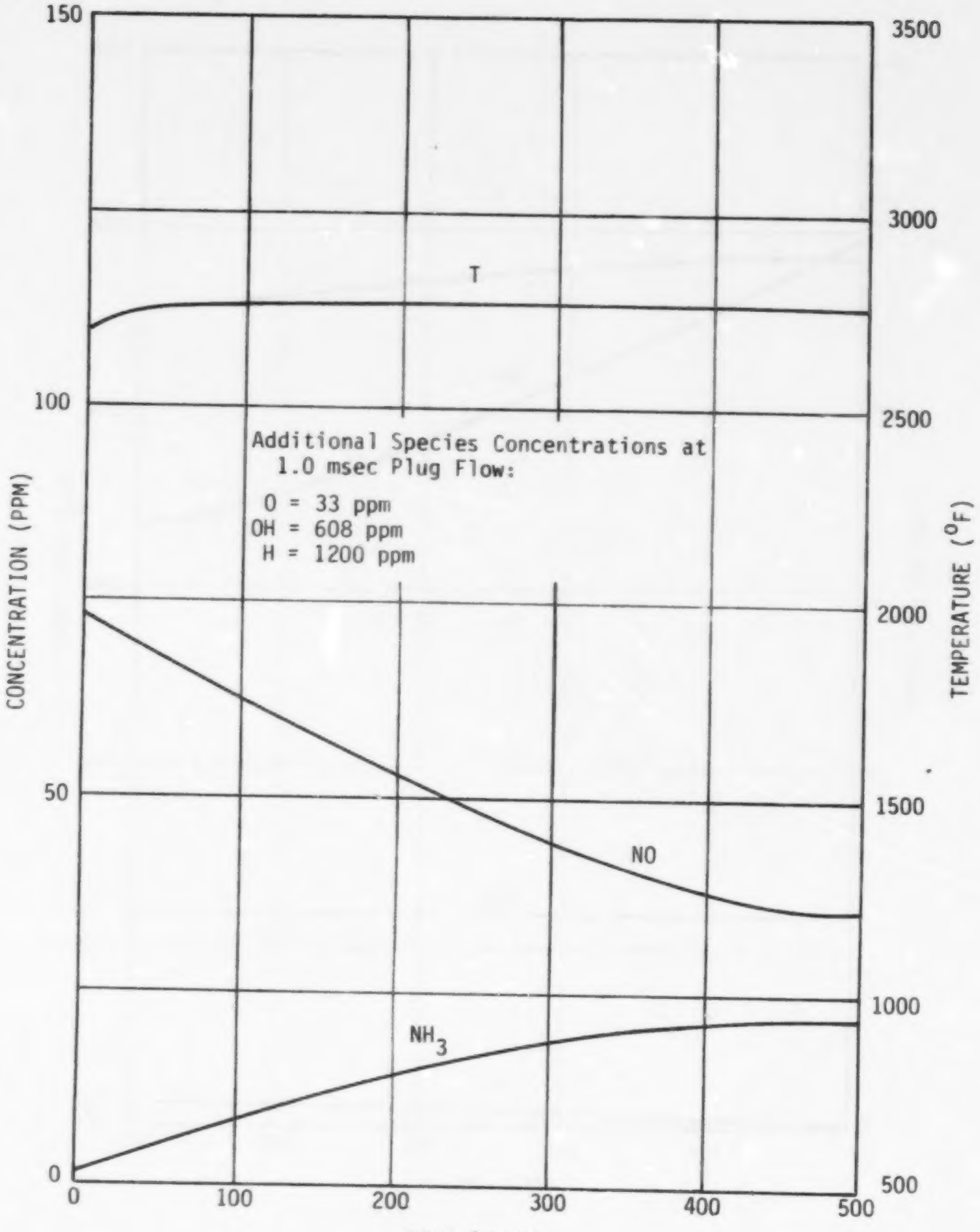


Figure 4-50. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: $\phi = 1.15$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; $(NH_3)_0 = 243$ ppm (500 ppm in fuel); Heat transfer = -71 Btu/lb (equivalent to -200^{o}F ΔT)



Additional Species Concentrations at 1.0 msec Plug Flow:

O = 33 ppm
OH = 608 ppm
H = 1200 ppm

Figure 4-51. Nitrogen Species and Temperature in Rich Primary Zone — Supercharged Boiler

NOTE: $\phi = 1.33$; Ordinate values from stirred reactor ignition zone $\tau_{SR} = 1.0$ msec; $(NH_3)_0 = 263$ (500 ppm in fuel); No heat transfer; No fuel methane (equivalent to $CH_4 + 1/2\ O_2 \rightarrow CO + 2H_2O$ proceeding instantaneously)

4.4.3.3 Secondary Stage — Distributed Heat Exchange and Energy Release

The rich primary stage discussed in the previous section serves two functions. First, it provides a means to partially control the fuel nitrogen conversion to NO_x, and second, it allows the subsequent staging of energy release (combustion air addition) and heat transfer to control thermal NO. This section presents the results of secondary stage calculations using the primary reactor data from the previous section as input. In all cases a primary reactor equivalence ratio of 1.15 was used since this was most effective in minimizing the effect of fuel nitrogen.

Figures 4-52 and 4-53 present species and temperature distributions for a 1.0 second residence time secondary stage. They differ only in the distribution of secondary air. In Figure 4-52 the air is added over 125 msec and in Figure 4-53 it is added over 500 msec. In both cases the primary residence time was taken as 500 msec and the primary zone heat loss corresponded to a 200°F drop in primary zone temperatures.

The heat transfer distribution is shown in the sketches on Figures 4-52 and 4-53 and has a peak-to-minimum heat flux ratio of 3:1 with the peak located at a point 25 percent of the length down the secondary combustor. This distribution was based on preliminary engineering estimates of radiative heat transfer. Perturbations on this distribution and on the required secondary residence time (as dictated by heat transfer limitations) were found to have little effect on the final NO level. Hence, refined heat transfer calculations were not performed.

With the air distribution in Figure 4-52, the NO level is relatively uneffected until the system leans out and the equivalence reaches 1.0 at approximately 100 msec into the system. At this point the remaining HCN rapdily converts to NO over a period of 50 msec and thermal NO production commences and continues until the temperature drops below the thermal threshold of 2700-2800°F which occurs 350 msec downstream. Further downstream the NO level remains constant at 110 ppm.

In Figure 4-53 the secondary air addition is delayed relative to Figure 4-52 and occurs uniformly over the first half of the combustor, thus reducing peak temperatures and eliminating thermal NO entirely. The NO level

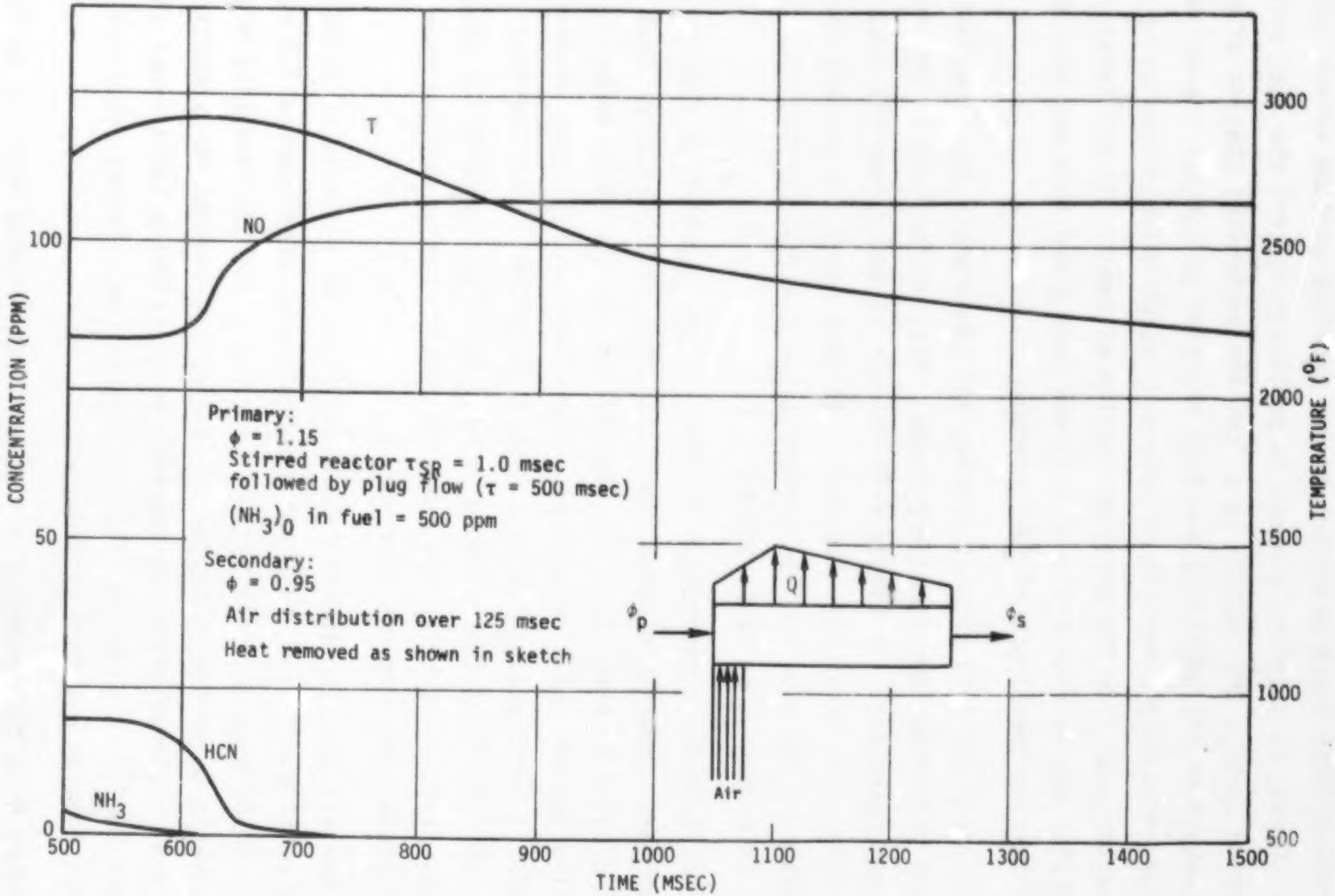
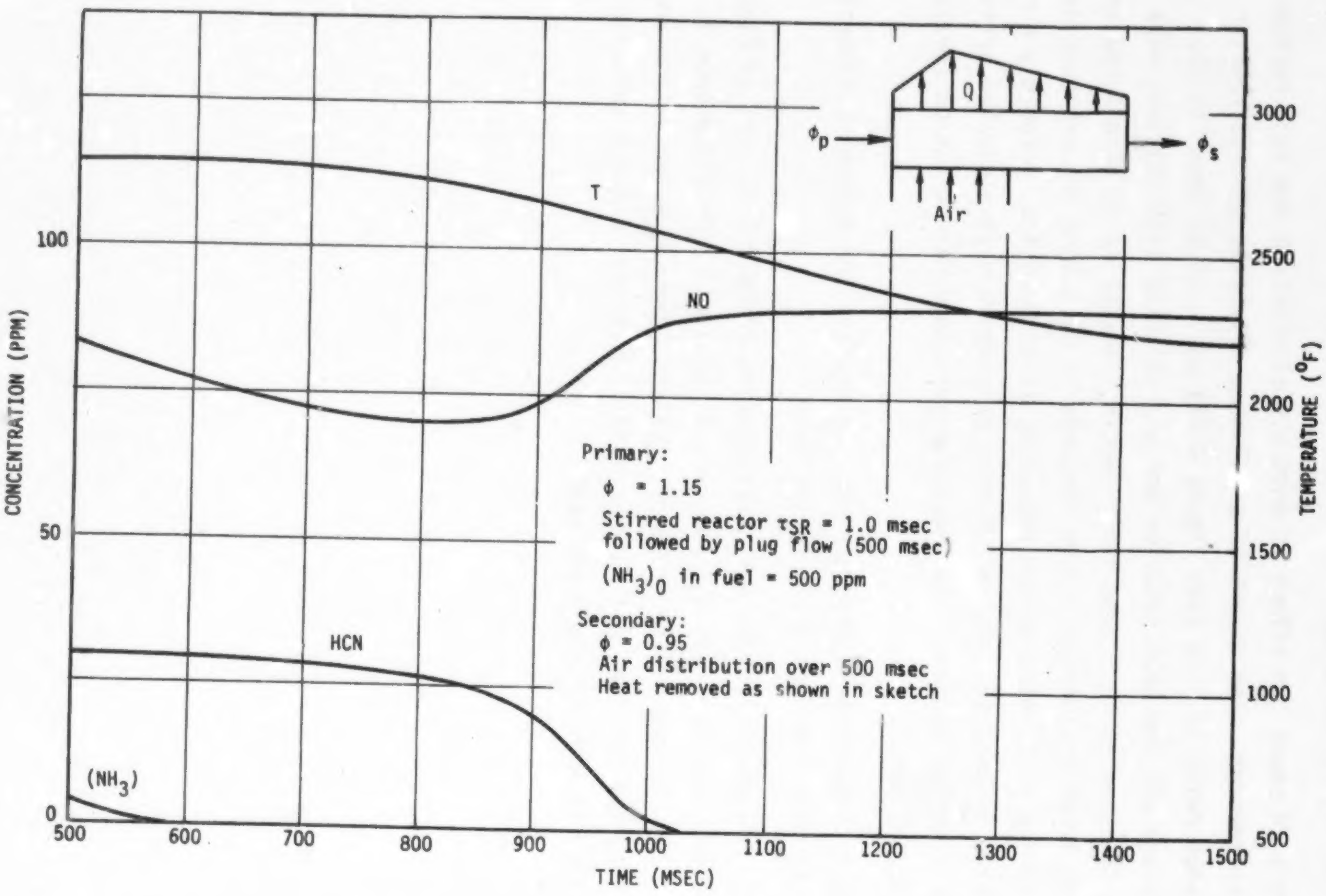


Figure 4-52. Nitrogen Species and Temperature in Secondary Stage — Supercharged Boiler — Air Added Over 125 msec



Primary:

ϕ = 1.15

Stirred reactor τ_{SR} = 1.0 msec followed by plug flow (500 msec)

$(NH_3)_0$ in fuel = 500 ppm

Secondary:
ϕ = 0.95
Air distribution over 500 msec
Heat removed as shown in sketch

Figure 4-53. Nitrogen Species and Temperature in Secondary Stage — Supercharged Boiler — Air Added Over 500 msec

at first decreases due to dilution and then increases to its final value of 90 ppm as the HCN is converted.

Figure 4-54 shows the effect of entirely eliminating the long residence time primary reactor. The output of a 1.0 msec adiabatic stirred reactor at an equivalence ratio of 1.15 (see Figure 4-41) was used as input to the secondary stage and the heat transfer and air addition distributions were maintained the same as in Figure 4-53. Again, thermal NO is eliminated and the final NO level is 150 ppm. Thus the benefit of a long primary cooking period is on the order of a 60 ppm reduction in NO emission. Probably a compromise design is best in which a 200 msec primary zone participates actively in the heat transfer process. Such a combustor would have emission levels on the order of 125 ppm.

Figure 4-55 combines a single plot, the primary and secondary distributions from Figures 4-50 and 4-52 respectively.

Finally, Figure 4-56 provides a calculation identical to that of Figure 4-54 except that the fuel NH_3 has been eliminated. The difference in NO levels following the stirred reactor persists throughout the system and indicates that the net fuel nitrogen contribution to the exhaust emissions in Figure 4-54 is approximately 100 ppm.

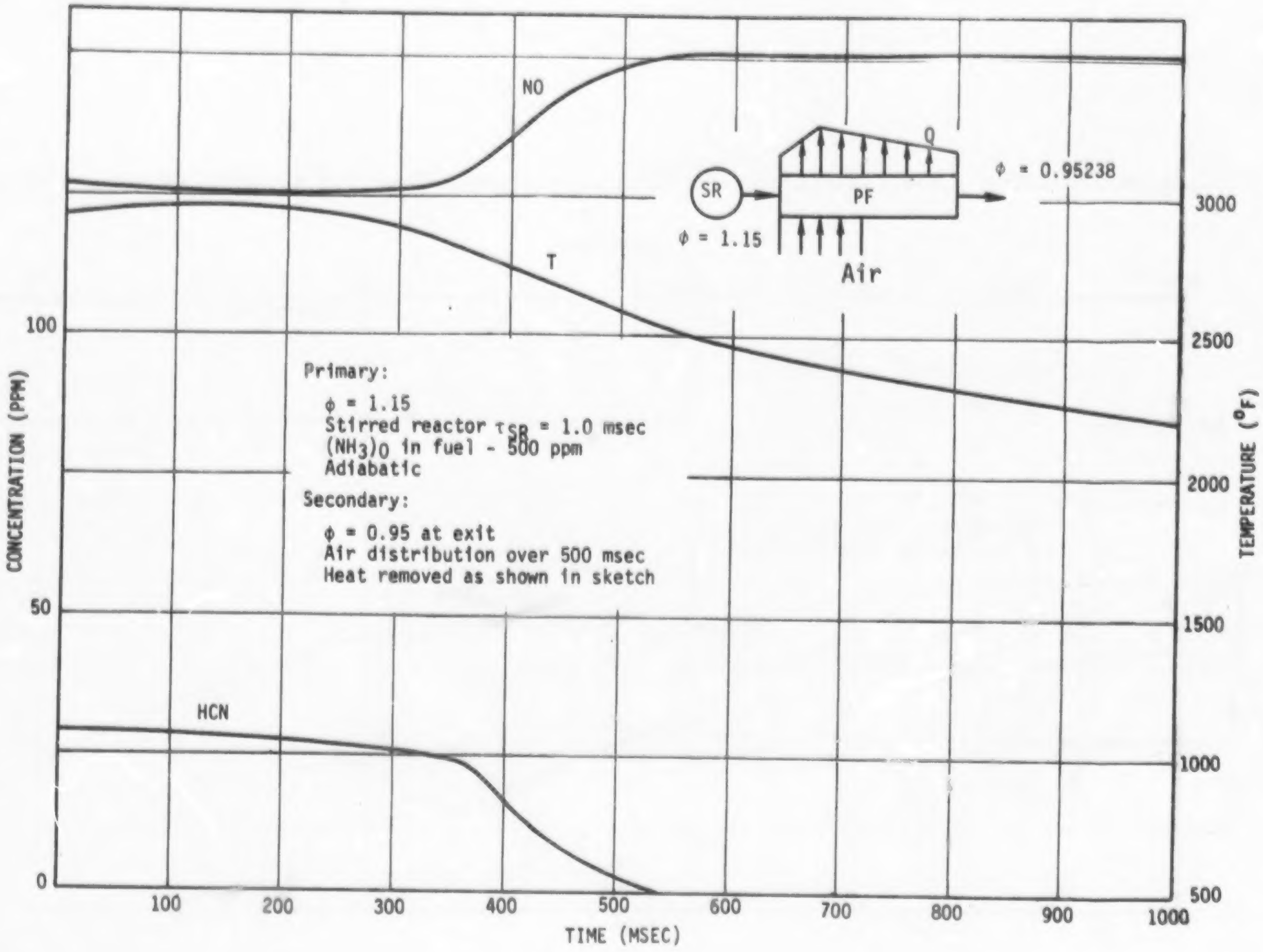
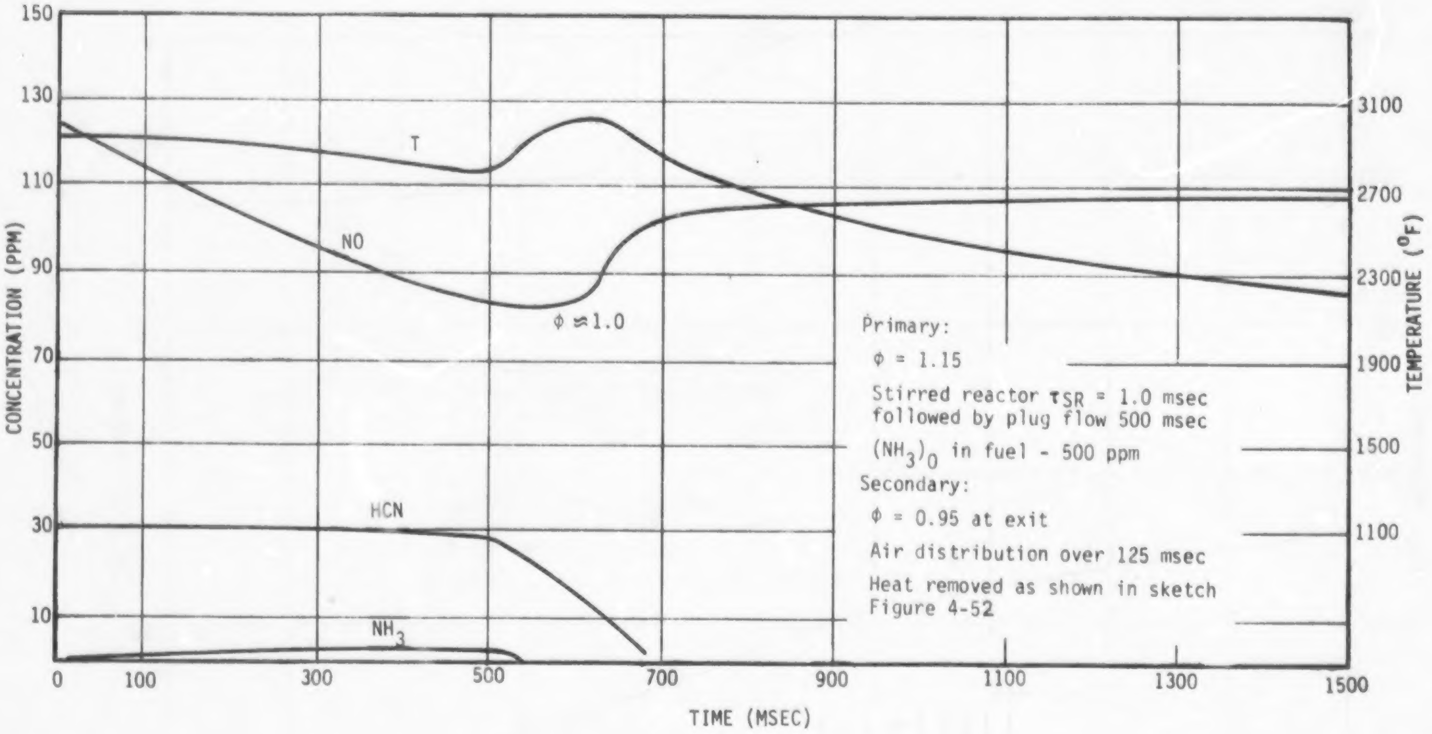


Figure 4-54. Nitrogen Species and Temperature in Secondary Stage — Supercharged Boiler — Stirred Reactor Primary Stage



Primary:

$\phi = 1.15$

Stirred reactor $\tau_{SR} = 1.0$ msec followed by plug flow 500 msec

$(NH_3)_0$ in fuel - 500 ppm

Secondary:

$\phi = 0.95$ at exit

Air distribution over 125 msec

Heat removed as shown in sketch Figure 4-52

Figure 4-55. Nitrogen Species and Temperature in Primary and Secondary Stage – Supercharged Boiler

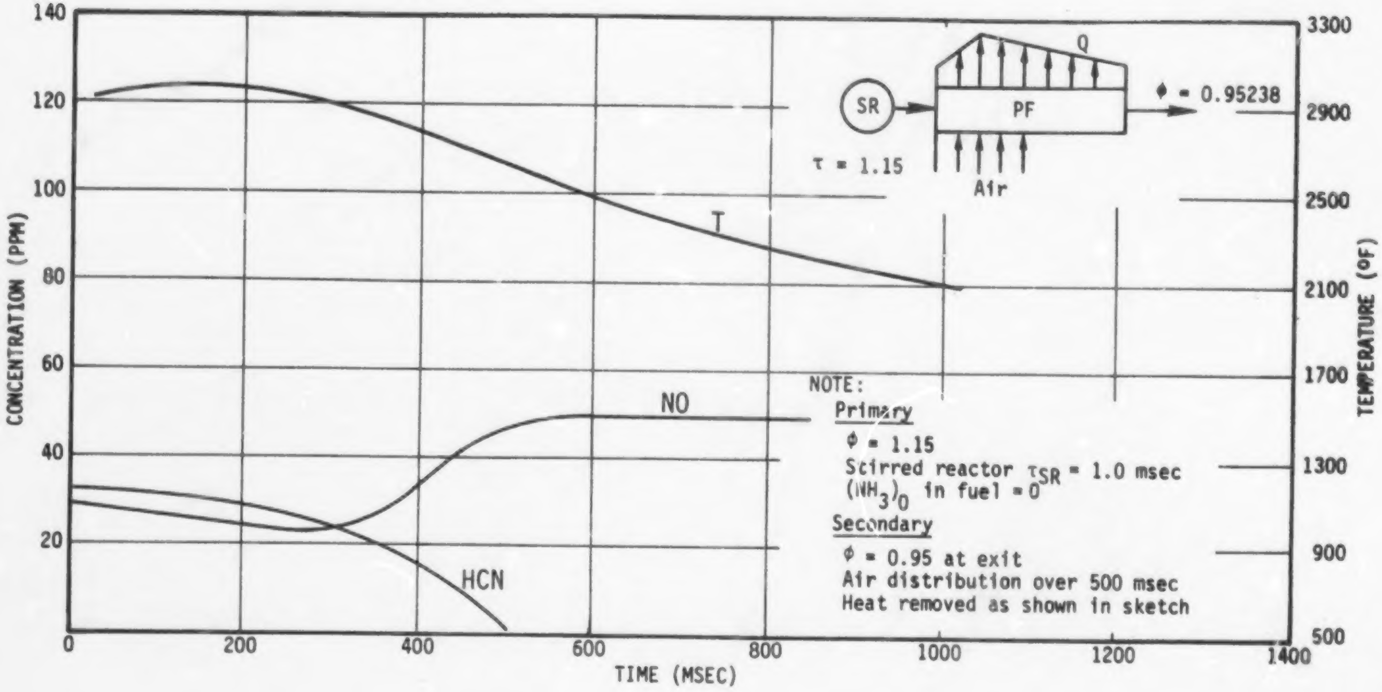


Figure 4-56. Nitrogen Species and Temperature in Secondary Stage — Supercharged Boiler

5.0 CONCLUSIONS

The major conclusions of this study were:

- A chemical kinetic reaction set is available which may be suitable for engineering calculations; however, it needs further validation, modification and reduction.
- Gasifier-COGAS systems appear to be potentially efficient energy conversion devices if developed as integrated systems.
- Low NO_x emission combustors can probably be developed without the need for NH_3 removal from the gasifier raw gas.

For both concepts studied it was found that careful combustor design can contribute significantly to reduction of NO_x emissions from low Btu gas systems. Staging the combustion process was found to be desirable in both cases.

The optimum design for an adiabatic gas turbine combustor was found to be a rich ($1.33 < \phi < 1.45$) primary reactor section with a residence time of at least 200 msec followed by a gradual mixing of the primary products into the dilution air stream. NO_x emissions for such a system could potentially be lower than those for an unstaged system by factors of five or more.

For the supercharged boiler case the optimum configuration consisted of a rich primary zone ($\phi=1.15$) and a secondary zone with gradual air introduction. The potential NO_x reduction compared with the unstaged configuration is a factor of three in this case.

Although this study considered only idealized combustor configurations and utilized a kinetic model that has not been completely validated, the results can be taken to indicate that there is an excellent likelihood that NO_x emissions from low Btu gas power generation systems can be held within acceptable limits. If validated, this conclusion will influence the need for high temperature ammonia cleanup.

It must be stressed that the calculations described in this report were made with the most appropriate reaction set available at that time and with full recognition of some of its deficiencies. Experimental evidence exists indicating that under certain conditions in premixed flames a large quantity of the NH_3 is converted to HCN prior to or coincident with the formation of

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NO or N_2. The current reaction set does not allow for this type of exchange nor is the oxidation of HCN adequately described.

One interesting observation is that for certain conditions (stoichiometry, time and temperature) final NO levels appear to be independent of the initial fuel nitrogen concentration. This observation is perhaps more relevant to other coal-derived fuels (e.g., liquids) with high nitrogen contents, and therefore, high NO emission potential. Suitable combustion chamber design can possibly overcome NO_x emission problems by maintaining rich products at relatively high temperatures to allow nitrogen fragments to equilibrate.

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APPENDIX A

ALTERNATIVE CONVENTIONAL AND COMBINED CYCLE SYSTEMS

This appendix gives the details of the conventional and combined cycle power generating systems investigated by Combustion Engineering as part of the preliminary screening process. See Section 2 for cycle comparisons.

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: A1

SYSTEM DESIGNATION: Conventional Utility Steam Power Plant

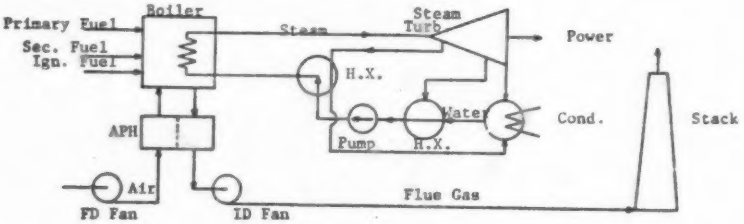
PRIMARY FUEL TYPE: Clean, low temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1 - Controlled circ; 2400 psia, 1005/1005°F, 3.5×10^6 lbm/hr main steam flow
  AIR PREHEATER: 2 - Ljungstrom
  BURNERS: C-E Type T (Tangential Firing)
  TURBINE–GENERATOR: Current designs; 500 MW (100%)

GAS TURBINE CYCLE:
  COMBUSTOR:
  TURBINE–GENERATOR:

NOx CONTROL: Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate
- All system components of current design
- Low NO_x potential
- Low operating cost
- High turndown ratio
- Conventional controls
- Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability)
- Retrofit of existing boiler practical
- Good system flexibility in following load demand (via primary fuel storage or secondary fuel capability)
- Potentially good system reliability

DISADVANTAGES:
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: A2

SYSTEM DESIGNATION: Conventional Utility Steam Power Plant

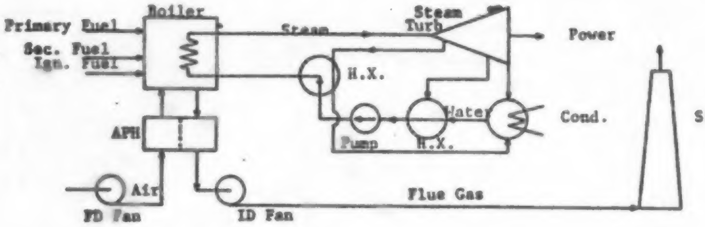
PRIMARY FUEL TYPE: Clean, low temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 1-Controlled circ; 2400 psia, 1005/1005°F; 3.5x10^6 lbm/hr main steam flow
AIR PREHEATER: 2-Ljungstrum
BURNERS: CE- Type T (Tangential Firing)
TURBINE–GENERATOR: Current designs; 500 MW (100%)

GAS TURBINE CYCLE:
COMBUSTOR:
TURBINE–GENERATOR:

NOx CONTROL: Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate
- All system components of current design.
- Low NOx potential
- Low operating cost
- High turndown ratio
- Convential controls
- Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability).
- Retrofit of existing boiler practical
- Good system flexibility in following load demand (via primary fuel storage or secondary fuel capacity.
- Potentially good system reliability.

DISADVANTAGES:

- High capital cost
- High pressure fuel more ideally suited to combined cycle applications.

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: B1

SYSTEM DESIGNATION: Conventional Utility Steam Plant with Gas Precooler

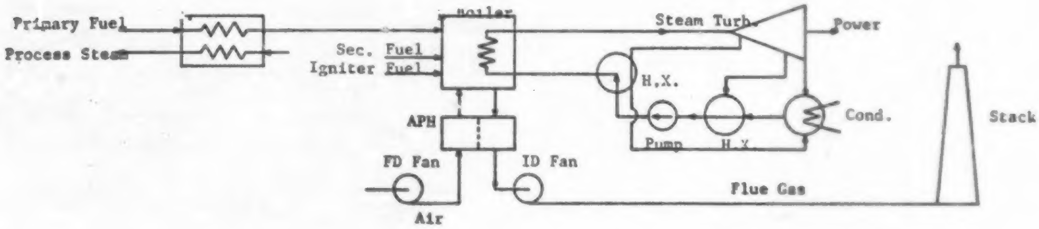
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1 - Controlled circulation; 2400 PSIA, 1005/1005°F; 3.5 x 10^6 lbm/hr main steam flow
  AIR PREHEATER: 2 - Ljungstrom
  BURNERS: C-E type T (Tangential Firing)
  TURBINE-GENERATOR: Current designs; 500 MW (100%)

GAS TURBINE CYCLE:
  COMBUSTOR:
  TURBINE-GENERATOR:

NOx CONTROL: Fuel Gas Precooling, Tangential Firing w/Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate
- All system components of current design
- Low NO_x potential
- Low operating cost
- High turndown ratio
- Conventional controls
- Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability)
- Retrofit of existing boiler practical
- Process steam produced for plant heating, auxiliaries, or power
- Good system flexibility in following load demand (via primary fuel storage or secondary fuel capability)
- Potentially good system reliability

DISADVANTAGES:
- High capital cost
- Heavily dependent on gas cooling for system availability
- Process steam flow dependent on plant load

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: B2

SYSTEM DESIGNATION: Conventional Utility Steam Plant w/Gas Precooler

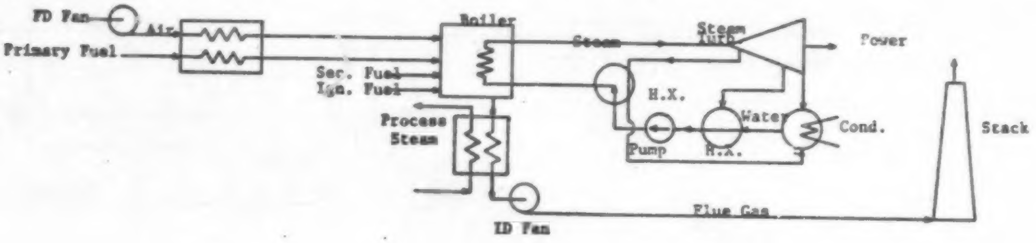
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas.

STEAM TURBINE CYCLE:
BOILER: 1 - Controlled circulation; 2400 PSIA, 1005/1005°F; 3.5 x 10^6 lbm/hr main steam flow
AIR PREHEATER: 2 recuperative
BURNERS: C-E Type T (Tangential Firing)
TURBINE-GENERATOR: Current designs; 500 MW (100%)

GAS TURBINE CYCLE:
COMBUSTOR:
TURBINE-GENERATOR:

NOx CONTROL: Fuel Gas Precooling, Tangential Firing w/Overfire Air, Flue Gas Recirculation

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate
- All system components of current design
- Low operating cost
- Very high turndown ratio
- Conventional controls
- Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability)
- Process steam produced for plant heating, auxiliaries or power
- Good system flexibility in following lead demand (via primary fuel storage or secondary fuel capability)
- Potentially good system reliability

DISADVANTAGES:
- High NO_x potential
- High capital cost
- Retrofit of existing boiler may not be practical
- Explosive potential of gas precooler

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: B3

SYSTEM DESIGNATION: Conventional Utility Steam Plant with Gas Precooler

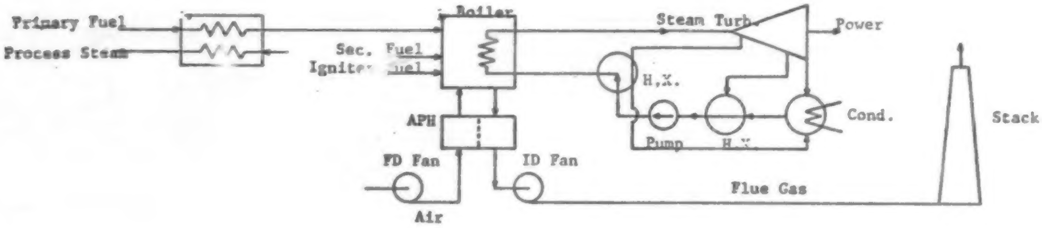
PRIMARY FUEL TYPE: Clean, high temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 1-Controlled circ; 2400 psia, 1005/1005°F; 3.5×10^6 lbm/hr main steam flow
AIR PREHEATER: 2-Ljungstrom
BURNERS: CE-Type T (Tangential Firing)
TURBINE-GENERATOR: Current designs; 500 MW (100%)

GAS TURBINE CYCLE:
COMBUSTOR:
TURBINE-GENERATOR:

NOx CONTROL: Fuel Gas Precooling, Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate
- All system components of current design
- Low NOx potential
- Low operating cost
- High turndown ratio
- Conventional controls
- Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability).
- Retrofit of existing boiler practical
- Good system flexibility in following load demand (via primary fuel storage or secondary fuel capabilit
- Potentially good system reliability.

DISADVANTAGES:
- High capital cost
- Heavily dependent on gas cooling for system availability
- Process steam flow dependent on plant load
- High pressure fuel more ideally suited to combined cycle applications.

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: C1

SYSTEM DESIGNATION: Conventional Utility Steam Plant w/High Temperature Burners

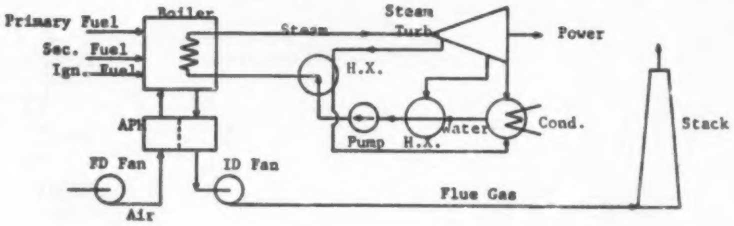
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1 - Controlled circulation; 2400 PSIA, 1005/1005°F; 3.5 x 10^6 lbm/hr main steam flow
  AIR PREHEATER: 2 - Ljungstrom
  BURNERS: High temperature Sulzer or new technology
  TURBINE–GENERATOR: Current designs, 500 MW (100%)

GAS TURBINE CYCLE:
  COMBUSTOR:
  TURBINE–GENERATOR:

NOx CONTROL: Overfire Air, FlueGas Recirc.

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate
- Low operating cost
- High turndown ratio
- Conventional controls
- Good system flexibility in following gasifier thruput (via secondary fuel capability)
- Retrofit of existing boiler practical
- Good system flexibility in following load demand (via secondary fuel capability)
- Potentially good system reliability.

DISADVANTAGES:
- Burner development may be required
- Very high NO_x potential
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: C2

SYSTEM DESIGNATION: Conventional Utility Steam Plant w/High Temperature Burners

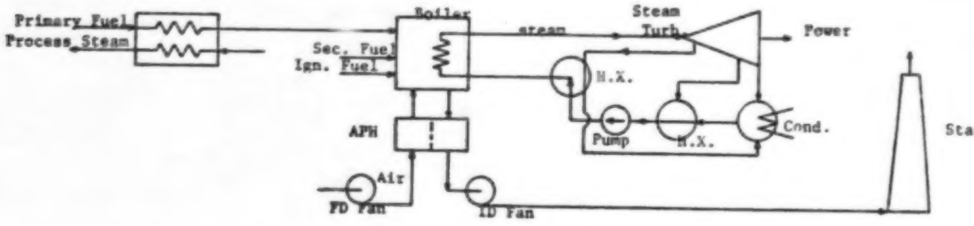
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1 - Controlled circulation; 2400 PSIA, 1005/1005°F; 3.5 x 10^6 lbm/hr main steam flow
  AIR PREHEATER: 2 - Ljungstrom
  BURNERS: High temperature Sulzer or New technology
  TURBINE-GENERATOR: Current designs; 500 MW (100%)

GAS TURBINE CYCLE:
  COMBUSTOR:
  TURBINE-GENERATOR:

NOx CONTROL: Overfire air; Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate
- Low operating cost
- High turndown ratio
- Conventional controls
- Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability)
- Retrofit of existing boiler practical
- Process steam produced for plant heating, auxiliaries, or power
- Good system flexibility in following load demand (via primary fuel storage or secondary fuel capability)
- Potentially good system reliability

DISADVANTAGES:
- Burner development may be required
- High NO_x potential
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: C3

SYSTEM DESIGNATION: Conventional Utility Steam Plant w/High Temperature Burners

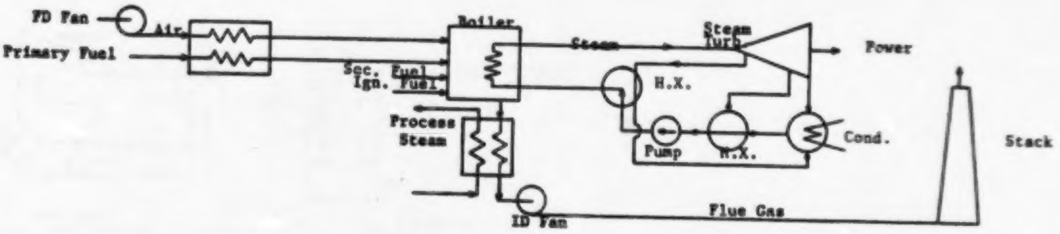
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1 - Controlled circulation; 2400 PSIA, 1005/1005°F; 3.5 x 10^6 lbm/hr main steam flow
  AIR PREHEATER: 2 - recuperative
  BURNERS: High temperature Sulzer or New technology
  TURBINE-GENERATOR: Current designs; 500 MW (100%)

GAS TURBINE CYCLE:
  COMBUSTOR:
  TURBINE-GENERATOR:

NO_x CONTROL: Overfire Air; Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:
- High turndown ratio
- Conventional controls
- Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability)
- Process steam produced for plant heating, auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage or secondary fuel capability)
- Potentially good system reliability

DISADVANTAGES:
- High plant net heat rate
- Burner development may be required
- High NO_x potential
- High capital cost
- High operating cost
- Explosive potential of gas precooler
- Retrofit of existing boiler may not be practical

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: D1

SYSTEM DESIGNATION: Industrial Boiler System

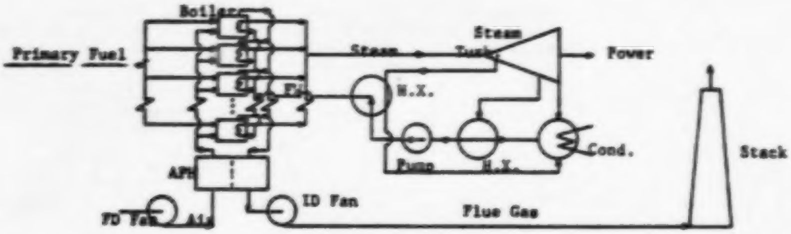
PRIMARY FUEL TYPE: Clean, low temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 11 - Natural circulation, shop assembled; 1800 psia 950°F; 0.4×10^6 lbm/hr steam flow
AIR PREHEATER: 2 - Ljungstrom
BURNERS: Front wall
TURBINE–GENERATOR: Current HP turbo design; possible new LP design; 500 MW (100%)

GAS TURBINE CYCLE:
COMBUSTOR:
TURBINE–GENERATOR:

NOx CONTROL: Overfire Air; Low excess air operation

SYSTEM SKETCH:



ADVANTAGES:
- All system components of current design
-
- Very high turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability)
- Good system flexibility in following load demand (via primary fuel storage or secondard fuel capability)
- Shop assembled boilers reduce load time for delivery

DISADVANTAGES:
- Very high plant net heat rate
- May require new steam turbine design
- High NO_x potential
- Very high operating cost
- Control system complexity
- Potentially poor system reliability
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: D2

SYSTEM DESIGNATION: Industrial Boiler System

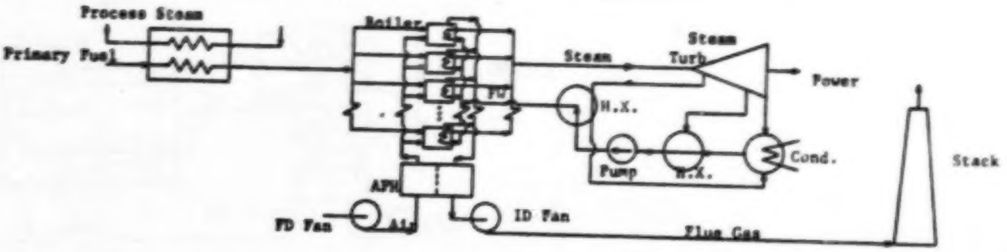
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 11-Natural circulation, shop assembled; 1800 psia, 950°F; 0.4×10^6 lbm/hr main stream flow
AIR PREHEATER: 2-Ljungstrom
BURNERS: Frontwall
TURBINE-GENERATOR: Current HP turb. design; possible new LP design ; 500 MW (100%)

GAS TURBINE CYCLE:
COMBUSTOR:
TURBINE-GENERATOR:

NOx CONTROL: Overfire Air; Low excess air operation.

SYSTEM SKETCH:



ADVANTAGES:
- -All system components of current design.
- -Process steam produced for plant heating, auxiliaries or power
- -Very high turndown ratio
- -Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability)
- -Good system flexibility in following load demand (via primary fuel storage or secondary fuel capability)
- -Shop assembled boilers reduce lead time for delivery

DISADVANTAGES:
- -Very high plant net heat rate
- -May require new steam turbine design
- -Very high operating cost
- -Control system complexity
- -Potentially poor system reliability
- -High NOx potential
- -High capital cost

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: D3

SYSTEM DESIGNATION: Industrial Boiler System

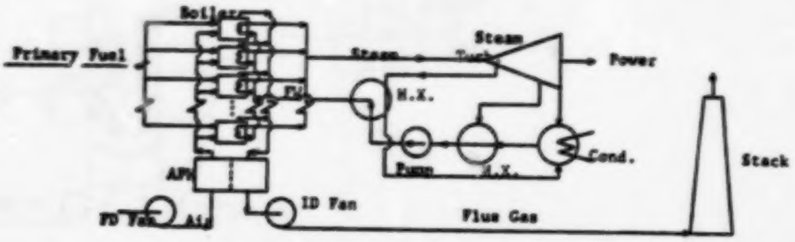
PRIMARY FUEL TYPE: Clean, low temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
    BOILER: 11-Natural circulation shop assembled; 1800 psia 950°F; 0.4x10^6 lbm/hr main steam flow
    AIR PREHEATER: 2-Ljungstrom
    BURNERS: Front wall
    TURBINE–GENERATOR: Current HP turb. design; possible new LP design; 500 MW (100%)

GAS TURBINE CYCLE:
    COMBUSTOR:
    TURBINE–GENERATOR:

NOx CONTROL: Overfire Air; low excess air operation

SYSTEM SKETCH:



ADVANTAGES:
- All system components of current design
- Low NOx potential
-
- Very high turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability)
- Good system flexibility in following load demand (via primary fuel storage or secondary fuel capability
- Shop assembled boilers reduce lead time for delivery

DISADVANTAGES:
- Very high plant net heat rate
- May require new steam turbine design
- Very high operating cost
- Control system complexity
- Potentially poor system reliability
- High pressure fuel more ideally suited to combined cycle applications
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: D4

SYSTEM DESIGNATION: Industrial Boiler System

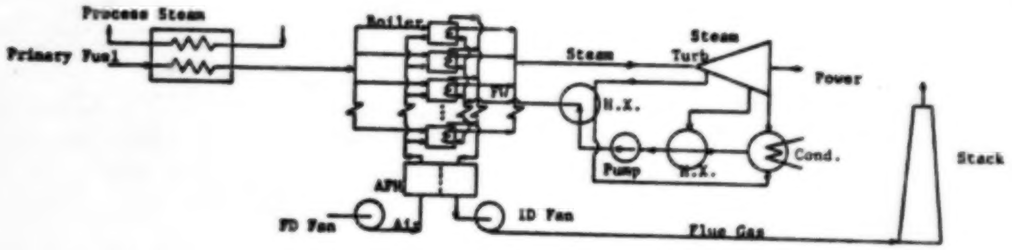
PRIMARY FUEL TYPE: Clean, high temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 11-Natural circulation, shop assembled; 1800 psia, 950°F; 0.4×10^6 lbm/hr main steam flow
AIR PREHEATER: 2-Ljungstrom
BURNERS: Front wall
TURBINE-GENERATOR: Current HP turb. design; possible new LP design; 500MW (100%)

GAS TURBINE CYCLE:
COMBUSTOR:
TURBINE-GENERATOR:

NOx CONTROL: Overfire Air; Low excess all operation

SYSTEM SKETCH:



ADVANTAGES:
- All system components of current design
-
- Very high turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage or secondary fuel capability).
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage or secondary fuel capability
- Shop assembled boilers reduce lead time for delivery

DISADVANTAGES:
- Very high plant net heat rate
- May require new steam turbine design
- Very high operating cost
- Control system complexity
- Potentially poor system reliability
- High pressure fuel more ideally suited to combined cycle applications
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: E1

SYSTEM DESIGNATION: Waste Heat Boiler Combined Cycle Plant

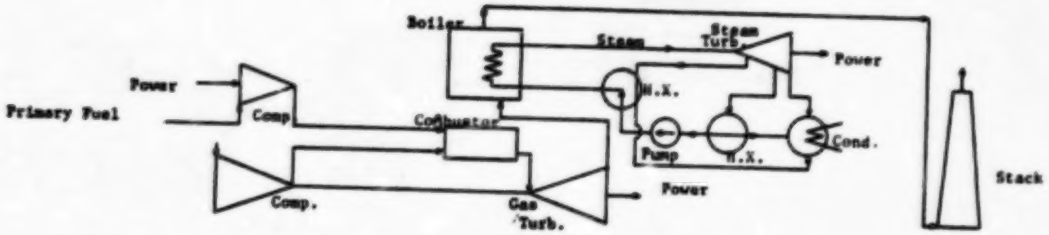
PRIMARY FUEL TYPE: Clean, low temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 5 - Natural circ.; 3 cycles to 1250 psia/1005°F (max.)
  AIR PREHEATER: -
  BURNERS: -
  TURBINE-GENERATOR: Current designs; 150 MW (30%)

GAS TURBINE CYCLE:
  COMBUSTOR: Current design
  TURBINE-GENERATOR: 5 sets; Current design ; 350 MW (70%)

NOx CONTROL: Water or steam injection to combustor.

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate
- All system components of current design
- Very high turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability
- Low operating cost

DISADVANTAGES:
- High NOx potential
- Control system complexity
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: E2

SYSTEM DESIGNATION: Waste Heat Boiler Combined Cycle Plant

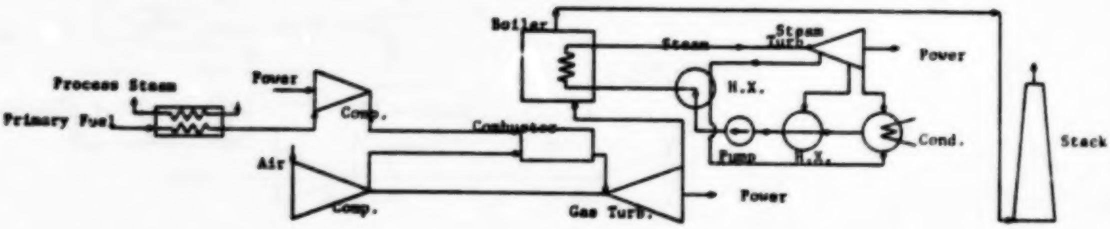
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 5 - Natural circ.; 3 cycles to 1250 psia/1005°F (max.)
  AIR PREHEATER: -
  BURNERS: -
  TURBINE-GENERATOR: Current designs; 150 MW (30%)

GAS TURBINE CYCLE:
  COMBUSTOR: Current design
  TURBINE-GENERATOR: 5 sets ; Current design ; 350 MW (70%)

NOx CONTROL: Steam or water injection to combustor.

SYSTEM SKETCH:


Boiler
Steam
Steam Turb.
Power
Process Steam
Power
Primary Fuel
Comp.
H.X.
Combustor
Pump
H.X.
Cond.
Stack
Air
Comp.
Gas Turb.
Power

ADVANTAGES:

- All system components of current design
- Low plant net heat rate

- Low operating cost
- Very high turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:

- High NOx potential
- Control system complexity
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: E3

SYSTEM DESIGNATION: Waste Heat Boiler Combined Cycle Plant

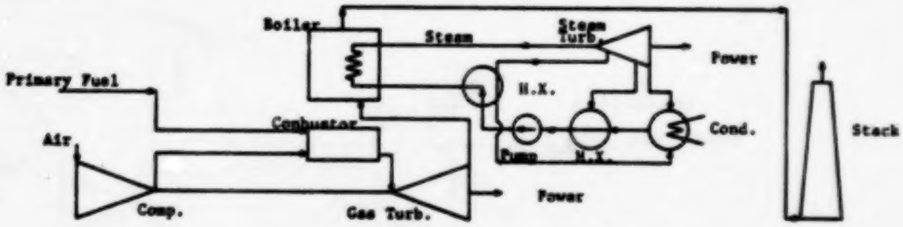
PRIMARY FUEL TYPE: Clean, low temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 5 - Natural circ.; 3 cycles to 1250 psia/1005°F (max.)
AIR PREHEATER:
BURNERS:
TURBINE-GENERATOR: Current designs; 150 MW (30%)

GAS TURBINE CYCLE:
COMBUSTOR: Current design
TURBINE-GENERATOR: 5 sets; Current design ; 350 MW (70%)

NOx CONTROL: Steam or water injection to combustor.

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate
- All system components of current design

- Low operating cost
- Very high turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- High NOx potential
- Control system complexity
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: E4

SYSTEM DESIGNATION: Waste Heat Boiler Combined Cycle Plant

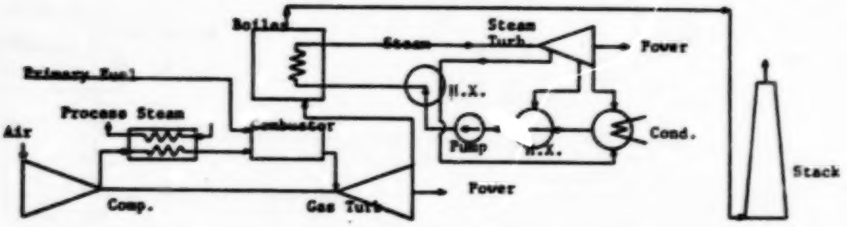
PRIMARY FUEL TYPE: Clean, high temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 5-Natural circ.; 3 cycles to 1250 psia/1005°F (max.)
  AIR PREHEATER:
  BURNERS:
  TURBINE-GENERATOR: 5 sets; Current design; 150 MW (30%)

GAS TURBINE CYCLE:
  COMBUSTOR: Current design
  TURBINE-GENERATOR: 5-sets, Current design; 350 MW (70%)

NOx CONTROL: Steam or water injection to combustor.

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate

- Low operating cost
- Very high turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- Combustor development may be required
- Very high NOx potential
- Control system complexity
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: E5

SYSTEM DESIGNATION: Waste Heat Boiler Combined Cycle Plant

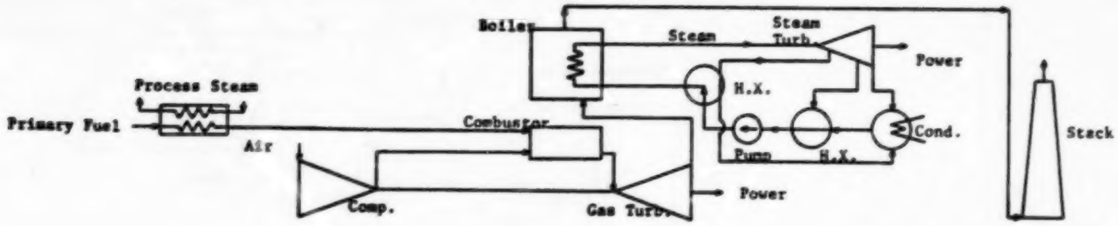
PRIMARY FUEL TYPE: Clean, high temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
- **BOILER:** 5- Natural circ.; 3 cycles to 1250 psia/1005°F (max.)
- **AIR PREHEATER:**
- **BURNERS:**
- **TURBINE-GENERATOR:** Current designs; 150 MW (30%)

GAS TURBINE CYCLE:
- **COMBUSTOR:** Current design
- **TURBINE-GENERATOR:** 5 sets; Current design; 350 MW (70%)

NOx CONTROL: Steam or water injection to combustor

SYSTEM SKETCH:



ADVANTAGES:
- Low plant net heat rate
- All system components of current design
- Very high turndown ratio

- Low operating cost
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- High NOx potential
- Control system complexity
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901801

SYSTEM CONCEPT NO: F1

SYSTEM DESIGNATION: Exhaust Fired Boiler Combined Cycle Plant

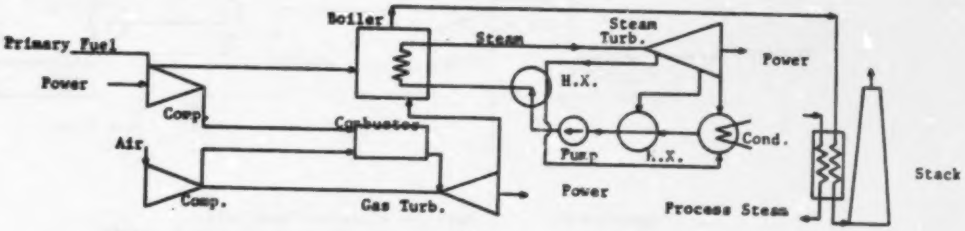
PRIMARY FUEL TYPE: Clean, low temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1-Controlled circ.; 2400 psia, 1005/1005°F; 2.8×10^6 lbm/hr main steam flow
  AIR PREHEATER:
  BURNERS: CE - Type T (Tangential Firing)
  TURBINE-GENERATOR: Current design; 400MW (80%)

GAS TURBINE CYCLE:
  COMBUSTOR: Current design
  TURBINE-GENERATOR: 2 sets; Current design; 100 MW (20%)

NOx CONTROL: Tangential Firing w/Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:


Boiler
Primary Fuel
Power
Comp
Combustor
Air
Comp.
Gas Turb.
Steam
Steam Turb.
Power
H.X.
Pump
H.X.
Cond.
Power
Process Steam
Stack

ADVANTAGES:
- Very low plant net heat rate
- All system components of current design
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901081

SYSTEM CONCEPT NO: F2

SYSTEM DESIGNATION: Exhaust Fired Boiler Combined Cycle Plant

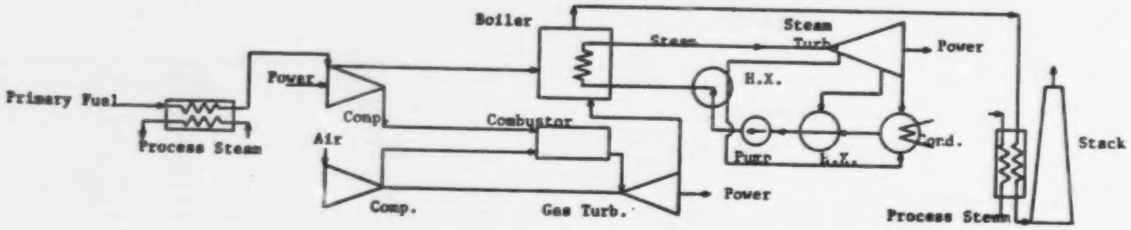
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 1-Controlled circ; 2400 psia, 1005/1005°F; 2.8×10^6 lbm/hg main steam flow
AIR PREHEATER:
BURNERS: CE - Type T (Tangential Firing)
TURBINE-GENERATOR: Current designs; 400MW (80%)

GAS TURBINE CYCLE:
COMBUSTOR: Current design
TURBINE-GENERATOR: 2-sets; Current design; 100 MW (20%)

NOx CONTROL: Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:


Boiler
Steam
Steam
Turb.
Power
Primary Fuel
Power
Comp.
H.X.
Combustor
Air
Process Steam
Pump
H.X.
Cond.
Stack
Comp.
Gas Turb.
Power
Process Steam

ADVANTAGES:
- Very low plant net heat rate
- All system components of current design
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- High capital cost
- Control system complexity
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: F3

SYSTEM DESIGNATION: Exhaust Fired Boiler Combined Cycle Plant

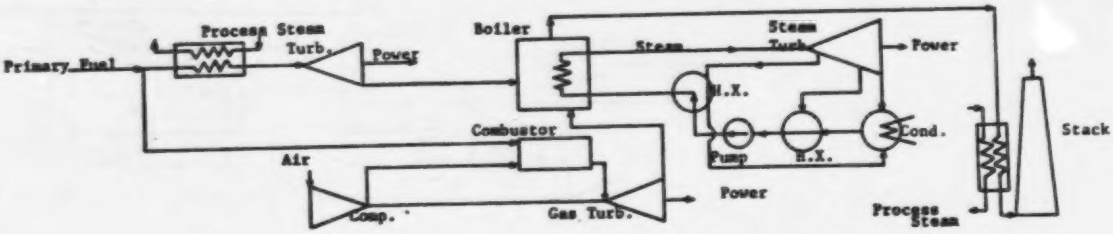
PRIMARY FUEL TYPE: Clean, low temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1-Controlled circ; 2400 psia, 1005/1005°F; 2.8×10^6 lbm/hr main steam flow
  AIR PREHEATER:
  BURNERS: CE-Type T (Tangential Firing)
  TURBINE-GENERATOR: Current designs; 400 MW (80%)

GAS TURBINE CYCLE:
  COMBUSTOR: Current design
  TURBINE-GENERATOR: 2-sets; Current design; 100MW (20%)

NOx CONTROL: Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:


Primary Fuel
Process Steam
Turb.
Power
Boiler
Steam
Steam Turb.
Power
H.X.
Pump
H.X.
Cond.
Stack
Combustor
Air
Comp.
Gas Turb.
Power
Process Steam

ADVANTAGES:
- Very low plant net heat rate
- All system components of current design
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901801

SYSTEM CONCEPT NO: F4

SYSTEM DESIGNATION: Exhaust Fired Boiler Combined Cycle Plant

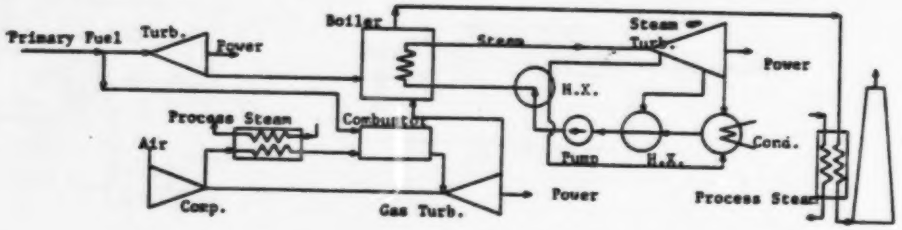
PRIMARY FUEL TYPE: Clean, high temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
- **BOILER:** 1-Controlled circ; 2400 psia, 1005/1005°F; 2.8×10^6 lbm/hr main steam flow
- **AIR PREHEATER:**
- **BURNERS:** Hi Temp. Sulzer or New Technology
- **TURBINE-GENERATOR:** Current designs; 400MW (80%)

GAS TURBINE CYCLE:
- **COMBUSTOR:** Current design
- **TURBINE-GENERATOR:** 2 sets; Current design; 100 MW (20%)

NOx CONTROL: Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:


Primary Fuel
Turb.
Power
Boiler
Steam
Steam Turb.
Power
H.X.
Process Steam
Combustor
Air
Pump
H.X.
Cond.
Stack
Comp.
Gas Turb.
Power
Process Steam

ADVANTAGES:
- Very low plant net heat rate
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- Burner development may be required
- High NOx potential
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: F5

SYSTEM DESIGNATION: Exhaust Fired Boiler Combined Cycle Plant

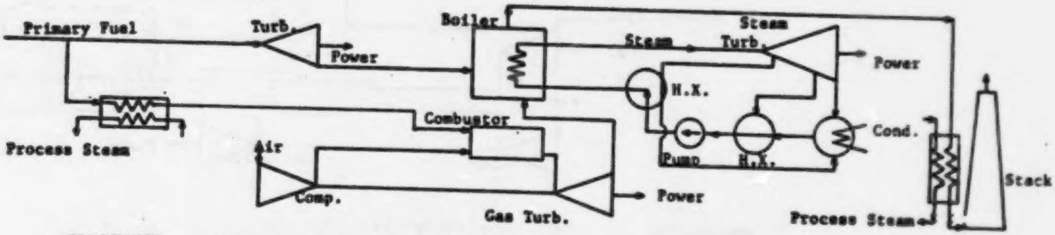
PRIMARY FUEL TYPE: Clean, high temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
- **BOILER:** 1-Controlled circ; 2400 psia, 1005/1005°F; 2.8x10^6 lbm/hr main steam flow
- **AIR PREHEATER:**
- **BURNERS:** CE-Type T (Tangential Firing)
- **TURBINE–GENERATOR:** Current designs; 400MW (80%)

GAS TURBINE CYCLE:
- **COMBUSTOR:** Current design
- **TURBINE–GENERATOR:** 2-sets; Current design; 100MW (20%)

NOx CONTROL: Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:


Primary Fuel
Turb.
Power
Boiler
Steam
Steam
Turb.
Power
H.X.
Combustor
Cond.
Process Steam
Air
Pump
H.X.
Comp.
Power
Gas Turb.
Stack
Process Steam

ADVANTAGES:
- Very low plant net heat rate
- All system componets of current design
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901081

SYSTEM CONCEPT NO: G1

SYSTEM DESIGNATION: Supplementary Fired Boiler Combined Cycle Plant

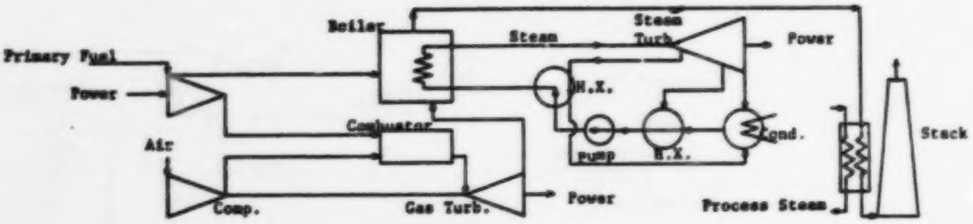
PRIMARY FUEL TYPE: Clean, low temperature , low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1-Controlled circ; 2400 psia, 1005/1005°F; 2.1×10^6 lbm/hr main steam flow
  AIR PREHEATER:
  BURNERS: CE-Type T (Tangential Firing)
  TURBINE-GENERATOR: Current designs; 300 MW (60%)

GAS TURBINE CYCLE:
  COMBUSTOR: Current design
  TURBINE-GENERATOR: 3-sets; Current design; 200 MW (40%)

NOx CONTROL: Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:
- Very low plant net heat rate
- All system components of current design
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: G2

SYSTEM DESIGNATION: Supplementary Fired Boiler Combined Cycle Plant

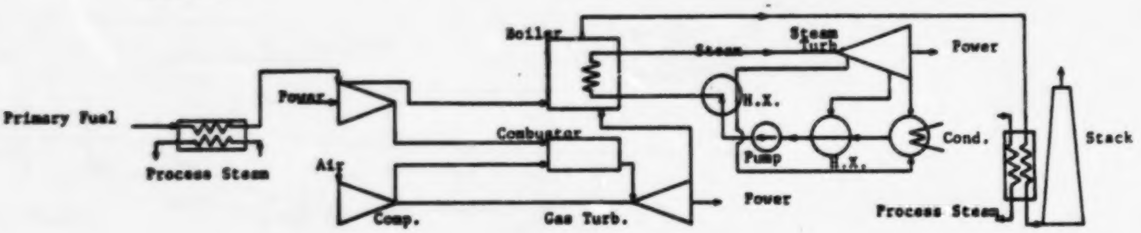
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 1-Controlled circ; 2400psia, 1005/1005°F; 2.1×10^{6} lbm/hr main steam flow
AIR PREHEATER:
BURNERS: CE-Type T (Tangential Firing)
TURBINE–GENERATOR: Current designs; 300 MW (60%)

GAS TURBINE CYCLE:
COMBUSTOR: Current design
TURBINE–GENERATOR: 3-sets; Current design; 200 MW (40%)

NOx CONTROL: Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:


Boiler
Steam Turb
Steam
Power
H.X.
Power
Primary Fuel
Combustor
Pump
H.X.
Cond.
Stack
Process Steam
Air
Power
Comp.
Gas Turb.
Process Steam

ADVANTAGES:
- Very low plant net heat rate
- All system components of current design
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: G3

SYSTEM DESIGNATION: Supplementary Fired Boiler Combined Cycle Plant

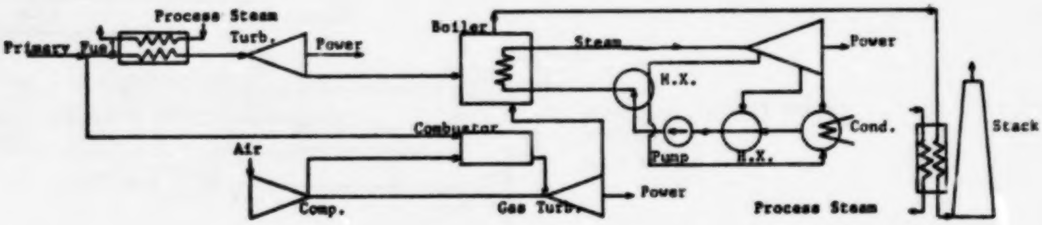
PRIMARY FUEL TYPE: Clean, low temperature, high pressure, low BTU gas.

STEAM TURBINE CYCLE:
  BOILER: 1-Controlled circ; 2400 psia, 1005/1005°F; 2.1×10^6 lbm/hr main steam flow
  AIR PREHEATER:
  BURNERS: CE-Type T (Tangential Firing)
  TURBINE–GENERATOR: Current designs; 300 MW (60%)

GAS TURBINE CYCLE:
  COMBUSTOR: Current design
  TURBINE–GENERATOR: 3-sets; Current design; 200 MW (40%)

NOx CONTROL: Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:


Process Steam
Primary Fuel
Turb.
Power
Boiler
Steam
Power
H.X.
Combustor
Air
Pump
H.X.
Cond.
Stack
Comp.
Gas Turb.
Power
Process Steam

ADVANTAGES:
- Very low plant net heat rate
- All system components of current design
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: G6

SYSTEM DESIGNATION: Supplementary Fired Boiler Combined Cycle Plant

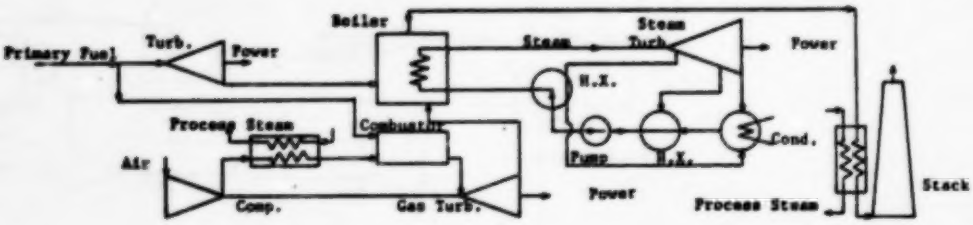
PRIMARY FUEL TYPE: Clean, high temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
- **BOILER:** 1-Controlled circ; 2400psia, 1005/1005°F; 2.1x10^6 lbm/hr main steam flow
- **AIR PREHEATER:**
- **BURNERS:** Hi Temp. Sulzer or New Technology
- **TURBINE-GENERATOR:** Current designs; 300 MW (60%)

GAS TURBINE CYCLE:
- **COMBUSTOR:** Current design
- **TURBINE-GENERATOR:** 3-sets; Current design; 200 MW (40%)

NOx CONTROL: Flue Gas Recirc.

SYSTEM SKETCH:


Boiler
Steam
Turb.
Primary Fuel
Turb.
Power
Steam
Power
H.X.
Process Steam
Combustor
Air
Cond.
Pump
H.X.
Stack
Comp.
Gas Turb.
Power
Process Steam

ADVANTAGES:
- Very low plant net heat rate
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- Burner development may be required
- Very high NOx potential
- Control system complexity
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901081

SYSTEM CONCEPT NO: G5

SYSTEM DESIGNATION: Supplementary Fired Boiler Combined Cycle Plant

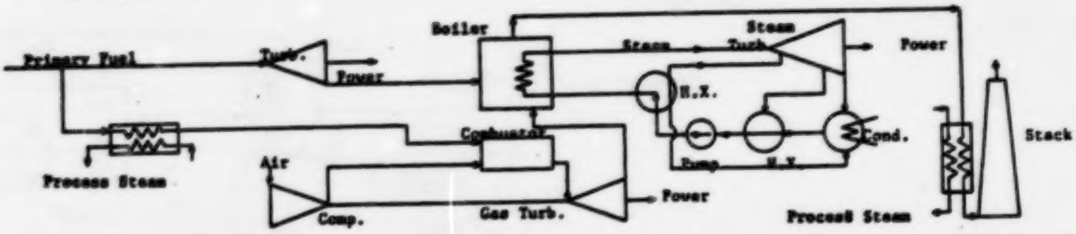
PRIMARY FUEL TYPE: Clean, high temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 1-Controlled circ; 2400 psia, 1005/1005°F; 2.1×10^6 lbm/hr main steam flow
AIR PREHEATER:
BURNERS: CE-Type T (Tangential Firing)
TURBINE-GENERATOR: Current designs; 300 MW (60%)

GAS TURBINE CYCLE:
COMBUSTOR: Current design
TURBINE-GENERATOR: 3-sets; Current design ; 200 MW (40%)

NOx CONTROL: Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:


Boiler
Steam
Steam Turb.
Power
Primary Fuel
Turb.
Power
H.X.
Combustor
Cond.
Stack
Pump
H.X.
Air
Process Steam
Power
Comp.
Gas Turb.
Process Steam

ADVANTAGES:
- Very low plant net heat rate
- All system components of current design
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating, auxiliaries or power
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: H1

SYSTEM DESIGNATION: Supercharged Boiler Combined Cycle

PRIMARY FUEL TYPE: Clean, low temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:

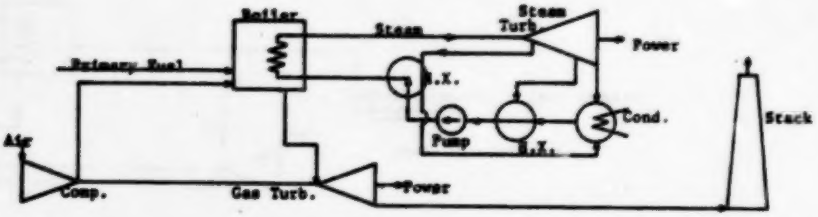
- **BOILER:** 1-Controlled circ; 2400 psia, 1005/1005°F; 2.8x10^{6} lbm/hr main steam flow
- **AIR PREHEATER:**
- **BURNERS:** CE-Type T (Tangential Firing)
- **TURBINE-GENERATOR:** Current designs; 400 MW (80%)

GAS TURBINE CYCLE:

- **COMBUSTOR:** Current design
- **TURBINE-GENERATOR:** 2-sets; Current designs; 100 MW (20%)

NOx CONTROL: Tangential Firing with Overfire Air, Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:

- Very low plant net heat rate
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Addition of process steam boiler or Gas turbine tail-end possible
- Low boiler size and heating surface requirements
- Good system flexibility in following load demand (via primary fuel storage or secondary fuel capability
- Potentially good system reliability

DISADVANTAGES:

- Boiler development required
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: H2

SYSTEM DESIGNATION: Supercharged Boiler Combined Cycle

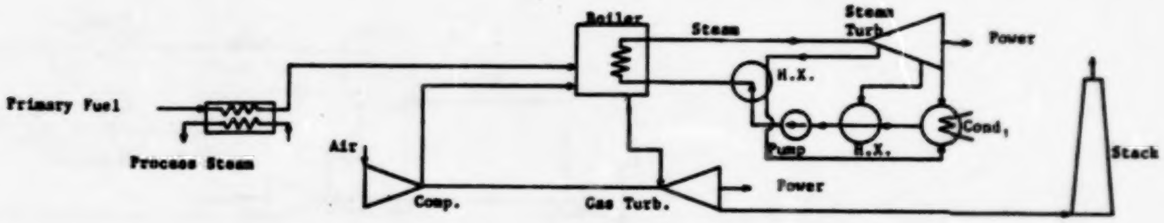
PRIMARY FUEL TYPE: Clean, high temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1-Controlled circ; 2400 psia, 1005/1005°F; $2.8x10^6$ lbm/hr main steam flow
  AIR PREHEATER:
  BURNERS: CE-Type T (Tangential Firing)
  TURBINE-GENERATOR: Current designs; 400 MW (80%)

GAS TURBINE CYCLE:
  COMBUSTOR: Current design
  TURBINE-GENERATOR: 2-sets; Current designs; 100 MW (20%)

NOx CONTROL: Tangential Firing with Overfire Air; Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:
- Very low plant net heat rate

- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Addition of process steam boiler or gas turbine tail-end possible
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- Boiler development required
- Control system complexity
- High capital cost

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: H3

SYSTEM DESIGNATION: Supercharged Boiler Combined Cycle

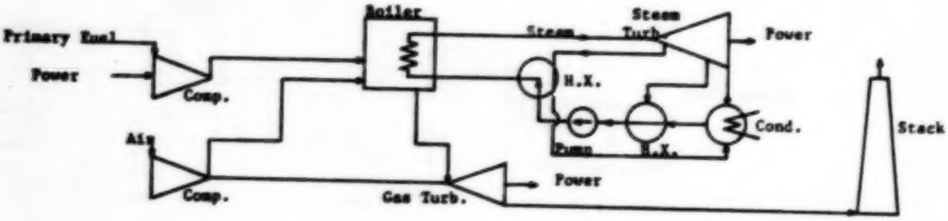
PRIMARY FUEL TYPE: Clean, low temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1-Controlled circ; 2400 psia, 1005/1005°F; 2.8x10^6 lbm/hr main steam flow
  AIR PREHEATER:
  BURNERS: CE-Type T (Tangential Firing)
  TURBINE-GENERATOR: Current designs; 400 MW (80%)

GAS TURBINE CYCLE:
  COMBUSTOR: Current design
  TURBINE-GENERATOR: 2-sets; Current designs; 100 MW (20%)

NOx CONTROL: Tangential Firing; with Overfire Air,; Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:
- Very low plant net heat rate
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Addition of process steam boiler on boiler or gas turbine tail-end possible
- Low boiler size and heating surface requirements
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:
- Boiler development required
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: IIA

SYSTEM DESIGNATION: Supercharged Boiler Combined Cycle

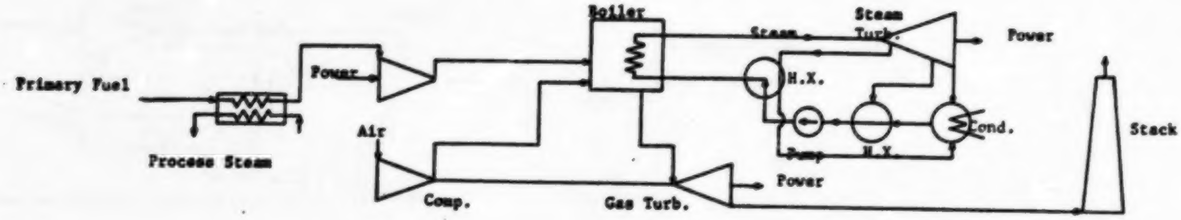
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 1-Controlled circ; 2400 psia, 1005/1005°F; 2.8×10^6 lbm/hr; main steam flow
AIR PREHEATER:
BURNERS: CE-Type T (Tangential Firing)
TURBINE-GENERATOR: Current designs; 400 MW (80%)

GAS TURBINE CYCLE:
COMBUSTOR: Current design
TURBINE-GENERATOR: 2-sets; Current designs; 100MW (20%)

NOx CONTROL: Tangential Firing with Overfire Air; Flue Gas Recirc.

SYSTEM SKETCH:



ADVANTAGES:

- Very low plant net heat rate
- Low NOx potential
- Low operating cost
- High turndown ratio
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Process steam produced for plant heating auxiliaries or power
- Addition of process steam boiler om boiler or gas turbine tail-end possible
- Low boiler size and heating surface requirements
- Good system flexibility in following load demand (via primary fuel storage)
- Potentially good system reliability

DISADVANTAGES:

- Boiler development required
- High capital cost
- Control system complexity

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: I1

SYSTEM DESIGNATION: O_2 Blown Supercharged Combined Cycle Plant

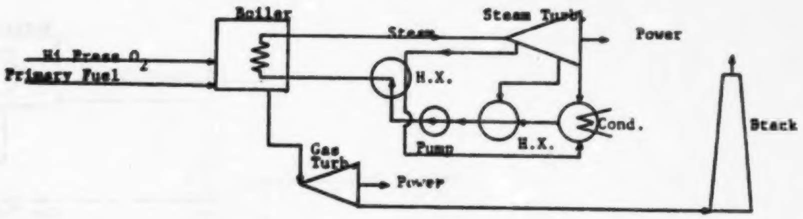
PRIMARY FUEL TYPE: Clean, low temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
- **BOILER:** 1-Controlled circ.; 2400 psia, 1005/1005°F; 2.8x10^6 lbm/hr main steam flow
- **AIR PREHEATER:**
- **BURNERS:** New Technology
- **TURBINE-GENERATOR:** Current design, 400 MW (80%)

GAS TURBINE CYCLE:
- **COMBUSTOR:**
- **TURBINE-GENERATOR:** 2-sets; Current designs; 100 MW (20%)

NOx CONTROL: O_2 blown

SYSTEM SKETCH:



ADVANTAGES:
- Very low plant net heat rate
- Very low NOx potential
- Low operating cost
- Good system flexibility in following gasifier thruput (via Primary fuel storage)
- Low boiler size and heating surface requirements
- Good system flexibility in following load demand (via primary fuel storage)

DISADVANTAGES:
- Burner development required
- Boiler development required
- High capital cost
- Unknown turndown ratio
- Control system complexity
- Applicability limited to O_2 blown gasifier
- Unknown system reliability
- Hi cost of O_2
- Applicability limited to N_2-free low BTU gas

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: I2

SYSTEM DESIGNATION: O_2 Blown Supercharged Steam Power Plant

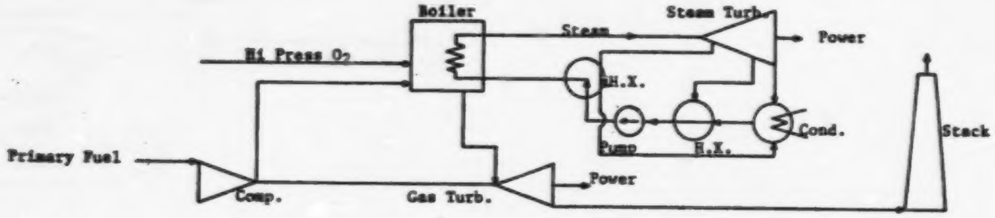
PRIMARY FUEL TYPE: Clean, low temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 1-Controlled circ.; 2400 psia, 1005/1005°F; 2.8×10^6 lbm/hr main steam flow
AIR PREHEATER:
BURNERS: New Technology
TURBINE-GENERATOR: Current design; 400 MW (80%)

GAS TURBINE CYCLE:
COMBUSTOR:
TURBINE-GENERATOR: 2-sets; Current designs; 100 Mw (20%)

NOx CONTROL: O_2 blown

SYSTEM SKETCH:



ADVANTAGES:

- Very low plant net heat rate
- Very low NOx potential
- Low operating cost
- Good system flexibility in following gasifier thruput (via primary fuel storage)
- Low boiler size and heating surface requirements
- Good system flexibility in following load demand (via primary fuel storage)

DISADVANTAGES:

- Burner development required
- Boiler development required
- High capital cost
- Unknown turndown ratio
- Control system complexity
- Poor system flexibility in following load demand (via primary fuel storage)
- Applicability limited to O_2 blown gasifier
- Unknown system reliability
- Hi cost of O_2
- Applicability limited to N_2-free low BTU gas

FURNACE DESIGN FOR BURNING OFFGAS FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: I3

SYSTEM DESIGNATION: O_2 Blown Supercharged Steam Power Plant

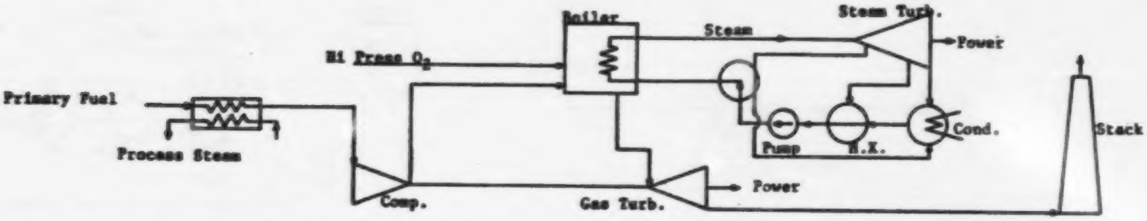
PRIMARY FUEL TYPE: Clean, high temperature, low pressure, low BTU gas

STEAM TURBINE CYCLE:
  BOILER: 1 Controlled circ.; 2400 psia, 1005/1005°F; 2.8×10^6 lbm/hr main steam flow
  AIR PREHEATER:
  BURNERS: New Technology
  TURBINE–GENERATOR: Current design; 400 MW (80%)

GAS TURBINE CYCLE:
  COMBUSTOR:
  TURBINE–GENERATOR: 2-sets; Current designs; 100 MW (20%)

NOx CONTROL: O_2 Blown

SYSTEM SKETCH:



ADVANTAGES:
- Very low plant net heat rate
- Low operating cost
- Process steam produced for plant heating auxiliaries or gasifier
- Low boiler size and heating surface requirements

DISADVANTAGES:
- Burner development required
- Boiler development required
- Very high NOx potential
- High capital cost
- Unknown turndown ratio
- Control system complexity
- Poor system flexibility in following primary fuel supply
- Poor system flexibility in following load demand
- Unknown system reliability
- Applicability limited to O_2 blown gasifier
- Hi cost of O_2
- Applicability limited to N_2-free low BSU gas.

FURNACE DESIGN FOR BURNING OFFGAS
FROM COAL GASIFIERS

TASK C
EPA CONTRACT 68-02-1361
CE CONTRACT 9673
PROJECT 901001

SYSTEM CONCEPT NO: I4

SYSTEM DESIGNATION: O_2 Blown Supercharged Combined Cycle Plant

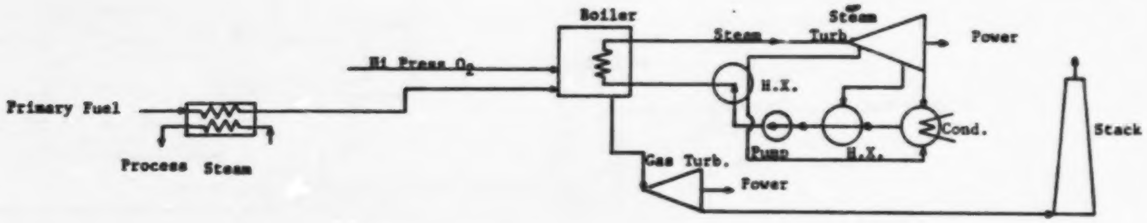
PRIMARY FUEL TYPE: Clean, high temperature, high pressure, low BTU gas

STEAM TURBINE CYCLE:
BOILER: 1-Controlled circ.; 2400 psia, 1005/1005°F; 2.8×10^6 lbm/hr main steam flow
AIR PREHEATER:
BURNERS: New Technology
TURBINE–GENERATOR: Current design; 400 MW (80%)

GAS TURBINE CYCLE:
COMBUSTOR:
TURBINE–GENERATOR: 2-sets; Current designs; 100 MW (20%)

NOx CONTROL: O_2 Blown

SYSTEM SKETCH:



ADVANTAGES:

- Very low plant net heat rate
- Low operating cost
- Process steam produced for plant heating auxiliaries or gasifier
- Low boiler size and heating surface requirements

DISADVANTAGES:

- Burner development required
- Boiler development required
- Very high NOx potential
- High capital cost
- Unknown turndown ratio
- Control system complexity
- Poor system flexibility in following primary fuel supply
- Poor system flexibility in following load demand
- Unknown system reliability
- Applicability limited to O_2 blown gasifier
- Hi cost of O_2
- Applicability limited to N_2-free low BTU gas

APPENDIX B

THE PREDICTION OF FURNACE PERFORMANCE FOR TANGENTIALLY-FIRED UTILITY BOILERS

Two requirements necessitated the development of an engineering model for predicting furnace performance in water-wall boilers. These are:

- The selection of the proper grade of steel for the water-wall requires a knowledge of axial heat absorption rate.
- The furnace outlet temperature must be known within about ±50°F in order to correctly size superheaters, reheaters and economizers.

The assessment of the performance of furnaces fired with low Btu gas described in Section 3 utilized Combustion Engineering's "lower furnace model". The development of this program was described by Bueters et al(20) and the region modeled by this program is shown in Figure B-1.

The furnace is divided into a number of horizontal strips as shown in Figure B-2. Heat absorption to the wall and the gas temperature in the exit plane are given by the simultaneous solution of an energy balance on each strip. This energy balance is given by

$$q_{iia} + q_i^1 + Q_i = q_{io_a} + q_{io}^1 + q_{io_r}$$

where

q_{iia} = axial radiation absorbed by slice i and emitted by all other slices

q_i^1 = sensible heat entering the ith slice

Q_i = heat released in the ith slice

q_{io_a} = axial emission of the ith slice

q_{io}^1 = sensible heat leaving the ith slice

q_{io_r} = radiation from the ith slice to its bounding wall

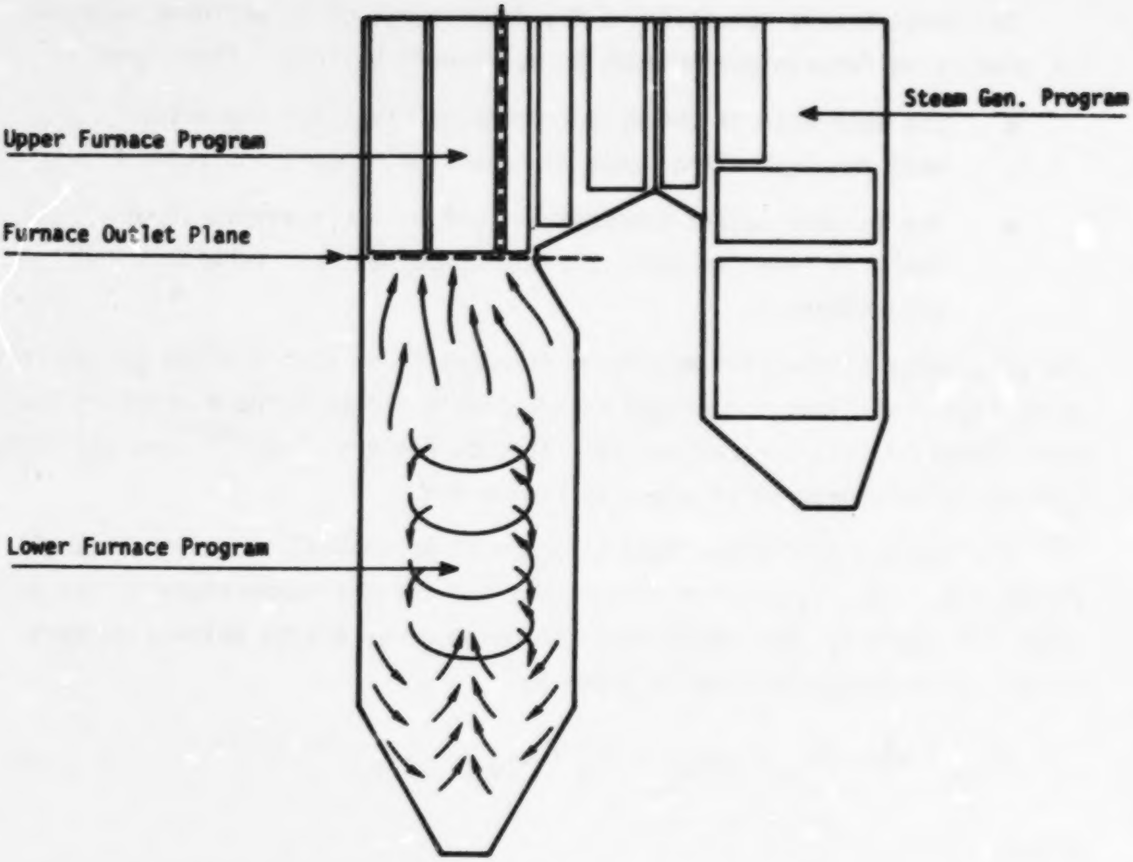
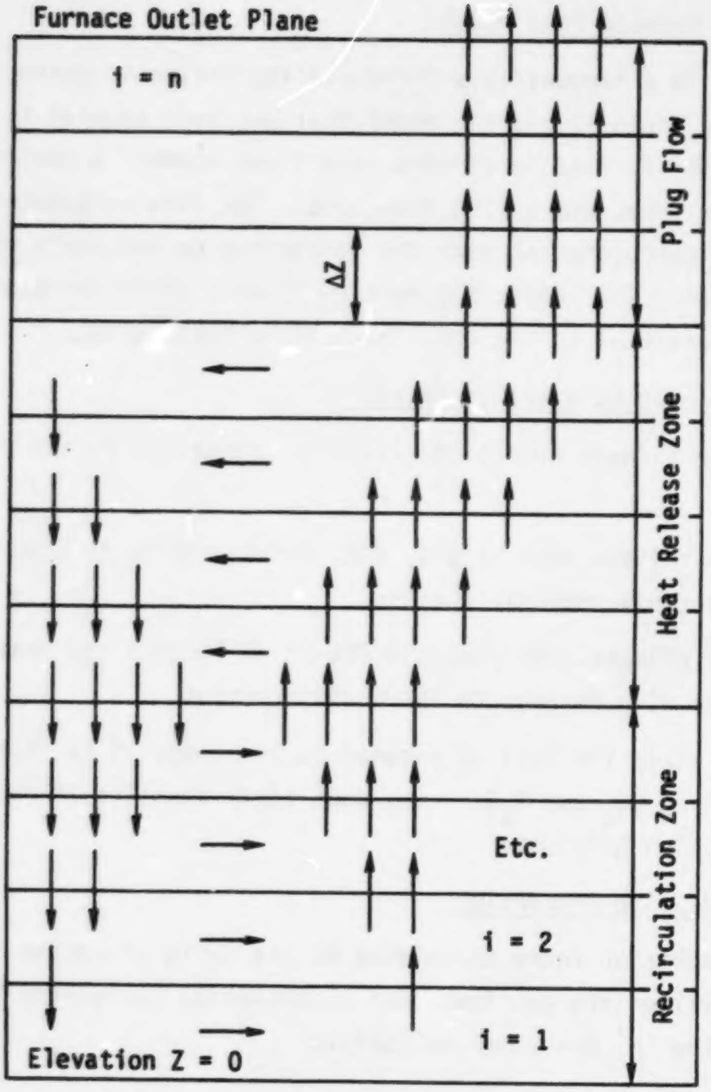

Upper Furnace Program
Furnace Outlet Plane
Lower Furnace Program
Steam Gen. Program

Figure B-1. Furnace Schematic Showing Volume Modeled by Lower Furnace Program


Furnace Outlet Plane
i = n
ΔZ
Plug Flow
Heat Release Zone
Recirculation Zone
Etc.
i = 2
i = 1
Elevation Z = 0

Lower Furnace Program Sample Gas Circulation Pattern

Figure B-2. Lower Furnace Program Recirculating Flow Model

The solution of this energy balance requires a description of:

- the furnace flow pattern,
- the heat release distribution,
- the radiative properties of the furnace gases, and
- the radiation exchange.

The Furnace Flow Model

The flow in a tangentially-fired utility boiler is characterized by a "donut" shaped fireball and the model that has been adopted is shown in Figure B-2. The furnace is divided into three zones: a recirculation zone, a heat release zone, and a plug flow zone. The flow originates in the heat release zone, circulates through the hopper region and peels off to rejoin the exit stream. The products generated in each strip are assumed to be directly proportional to the heat released in that strip.

The Heat Release Distribution

The lower furnace source condition is prescribed by two empirical parameters:

- The release zone height, RZH, (heat release is assumed uniform over this region), and
- The release zone centroid RZC which locates the heat release zone with respect to the furnace bottom.

In each strip the heat is assumed to be liberated instantaneously with the fuel forming CO_2 and H_2O. Thus each strip consists of fully-mixed, fully-burned combustion products.

Radiation Properties

Heat absorption rates calculated on the basis of carbon dioxide and water vapor emissivities are too low. Gas emissivities calculated from charts are modified by the "F_E Operator" as follows:

$$\bar{\varepsilon} = (F_E - 1 + \bar{\varepsilon}_H)/F_E$$

where $\bar{\varepsilon}_H$ is the combined emissivity of CO_2 and H_2O for the appropriate partial pressures and path length and the wall-to-gas and gas-to-gas absorptivities are similarly modified:

$$\alpha = (F_E - 1 + \alpha_H)F_E$$

Values of F_E have been determined for gas, oil and coal-firing and include corrections for soot radiation and convection.

Radiation Exchange

The "lower furnace program" allows for axial exchange between strips, but each strip only radiates to its own bounding surface wall.

Bueters, Cogoli and Habelt(20) have described the development of the "lower furnace program" in detail and show comparisons between measured and calculated absorption rates and furnace exit temperatures.

APPENDIX C

KINETIC MECHANISM OF NO_x FORMATION IN LOW BTU GAS COMBUSTION

C.1 INTRODUCTION

As the systems study progressed, it became increasingly obvious that accurate estimates of NO formation in supercharged boiler-combined cycle systems burning low Btu gas would not be possible. Consequently, it was decided to approach the problem by constructing limit-case models. These models are based upon the conjecture that chemical kinetics set the limit of NO production, but than in practice, emissions are dictated by mass transfer. Consequently, for the limit-case idealized mixing is assumed and constraints are imposed upon the system (inlet conditions, heat loss rate, residence time, exit temperature) corresponding to practical conditions. An essential feature of this model is the availability of a kinetic mechanism for NO formation.

Two factors make it necessary to synthesize a new kinetic mechanism capable of describing NO formation in low Btu gas combustion:

1. The presence of hydrocarbon species. Most coal-derived fuel gases will probably contain hydrocarbons (mainly methane), in addition to carbon monoxide and hydrogen.
2. The presence of ammonia. The yield of NO from ammonia in flames is strongly dependent upon the mixture equivalence ratio. In fuel-lean mixtures almost 100 percent of the ammonia is converted to NO, however, the conversion rate decreases significantly as the mixture become more fuel-rich.

C.2 NO FORMATION IN GASEOUS SYSTEMS

Nitric oxide can be formed from two nitrogen sources during the combustion of coal-derived fuel gases:

- Molecular nitrogen producing thermal NO
- Reduced nitrogen compounds (NH_3, HCN) producing fuel NO.

Experimental observations have characterized the most significiant features of nitric oxide formation from both sources.

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C.2.1 Thermal NO

Considerable effort has been expended in recent years to establish the kinetic mechanism which describes thermal NO formation in flames. In the post-flame gases, in regions far removed from the reaction zone, observed NO production rates can be explained on the basis of the Zeldovich mechanism(1). However, in regions close to the flame front, NO production rates exceed those predicted by the Zeldovich mechanism if equilibration of oxygen atoms is assumed. Two explanations have been proposed to account for this rapid formation of NO in, or close to, the flame front: non-equilibrium of oxygen atoms (O atom overshoot), and the attack of hydrocarbon radicals on nitrogen compounds, producing CN or NH type radicals. Both explanations are valid, but neither is exclusive. Oxygen atom overshoot does occur, but there is irrefutable evidence that hydrocarbon fuel fragments rupture nitrogen molecules producing nitrogen intermediates.

Fenimore(2) used the term "prompt" NO to describe the rapid formation of thermal NO in the flame front, and postulated two likely reactions involving nitrogen and fuel fragments which would produce intermediates which could then be converted to NO:

$$CH + N_2 \rightarrow CHN + N$$

$$C_2 + N_2 \rightarrow CN + CN$$

The existence of nitrogen intermediates in hydrocarbon flame fronts has been confirmed by De Soete(1), Eberius(3), and Haynes(4). These investigators report the presence of both HCN and "NH_i" in hydrocarbon flames.

C.2.2 Fuel NO

Several studies have been conducted in which simple nitrogen compounds were added to both premixed flames(1,5), and well-stirred reactors(6), in order to investigate the effect of temperature, pressure, fuel type, nitrogen, additive, additive concentration and equivalence ratio on fuel NO formation. Summarizing the most significant results of these investigations it appears that:

- Reaction zone equivalence ratio is the most important parameter controlling fuel NO formation.

- Compounds containing NH bonds tend to give higher conversion rates than compounds containing CN bonds in lean mixtures. However, in rich mixtures the conversion appears to be almost independent of the type of nitrogen compound.
- Conversion decreases as the concentration of nitrogen additive increases, and this effect is most apparent for fuel-rich mixtures.
- Flame temperature always has a relatively small influence on the formation of fuel NO, but it is enhanced for rich mixtures and additives with CN bonds.
- Fuel NO formation appears to be higher in rich hydrogen flames than in rich hydrocarbon flames.
- Pressure does not appear to have a very significant effect upon fuel NO formation.

It appears that the formation of fuel NO can be characterized by a rather simplistic view. The initial fuel nitrogen compound breaks down in the reaction zone producing an intermediate nitrogen compound XN. This XN intermediate is then subject to two competitive reaction paths:

Path A $XN + R'O \rightarrow NO + \ldots.$

Path B $XN + R''N \rightarrow N_2 + \ldots.$

Path A produces NO and is the faster of the two paths in lean mixtures. However, Path B dominates in fuel-rich mixtures, allowing the formation of molecular nitrogen. It can be seen that some similarity exists between the formation of fuel NO and the formation of prompt thermal NO by fuel fragments. XN intermediaries are produced by fuel fragments which are free to react through either Path A or Path B.

Path B allows the reduction of an intermediate compound XN to nitrogen. It is also known that NO itself behaves as a fuel nitrogen compound. Thus, NO can be reduced by R"N (Path B), or it can be converted to a nitrogen-containing intermediate. One possibility for the reduction of NO is the reverse of the first step of the Zeldovich mechanism

$$NO + N \rightarrow N_2 + O$$

Myerson(7) has indicated another route which will eventually allow the formation of N_2 from NO. He observed that hydrocarbon addition to simulated combustion products containing NO and oxygen caused a significant reduction in NO which he attributed to the occurrence of such reactions as

$$CH + NO \rightarrow HCN + O$$

$$CH + NO \rightarrow HCO + N$$

C.3 SYNTHESIS OF A REACTION SET

The kinetic mechanism synthesized for use in the estimation of NO formation in combustors burning low Btu gas should include the following features:

1. The ability to predict thermal NO formation and to take account not only of the Zeldovich mechanism, but also the formation of nitrogen intermediates produced by the reaction of fuel fragments.
2. The ability to be able to predict correctly the conversion of ammonia to NO and the destruction of NO by fuel-rich mixtures.
3. The reaction set should not be restricted to carbon monoxide and hydrogen since many coal-derived fuels contain hydrocarbons. Reaction involving higher hydrocarbons than methane were not to be included.

The majority of the reactions which were included had been listed by Engleman(8). The reaction set contains 27 species and 100 reactions. The total number of reactions are listed in Table C-1 in four groups:

- reactions describing the CH_4 oxidation mechanism
- reactions involving N, NO, N_2O or NO_2
- reactions of ammonia and intermediates
- reactions between carbon, hydrogen and nitrogen.

The reaction rate is expressed by

$$k_f = AT^{-N}e^{-E/RT}$$

Table C-1

$$k_f = AT^{-N} \exp(-E/RT)$$

REACTIONS DESCRIBING CH_4 OXIDATION MECHANISM

	A (cc, mole, sec)	N	E (kcal)	Ref.
$CH_4 + M = CH_3 + H + M$	2.00 E + 17	0.0	88.0	8
$CH_3O + M = CH_2O + H + M$	4.00 E + 40	7.5	22.6	10
$CH_2O + M = CHO + H + M$	8.00 E + 33	4.5	87.0	10
$CHO + M = CO + H + M$	2.50 E + 20	1.5	16.8	10
$CO_2 + M = CO + O + M$	1.00 E + 15	0.0	100.0	8
$H_2 + M = H + H + M$	2.00 E + 14	0.0	96.0	8
$H_2O + M = HO + H + M$	3.00 E + 15	0.0	105.0	11
$H + O + M = OH + M$	8.00 E + 15	0.0	0.0	8
$H + O_2 + M = HO_2 + M$	1.50 E + 15	0.0	1.0	8
$CH + CH_4 = CH_2 + CH_3$	1.00 E + 12	0.0	17.1	10
$CH + CH_3 = CH_2 + CH_2$	3.20 E + 12	0.0	8.0	10
$CH + HO = CHO + H$	5.00 E + 11	-0.5	10.0	8
$CH_3 + OH = CH_2 + H_2O$	1.00 E + 12	-0.7	2.0	8
$CH_2 + H_2 + CH_3 + H$	3.00 E + 12	0.0	7.0	10
$CH_3 + CH_2O = CH_4 + CHO$	4.00 E + 10	0.0	0.0	8
$CH_2 + CH_2O = CH_3 + CHO$	2.00 E + 11	0.0	6.5	10
$CH_2 + H = CH + H$	3.00 E + 11	-0.7	26.0	11
$CH_4 + OH = CH_3 + H_2O$	3.00 E + 13	0.0	5.0	8
$CH_4 + H = CH_3 + H_2$	5.00 E + 10	-1.0	10.0	11
$CH_4 + O = CH_3 + HO$	1.00 E + 10	-1.0	8.0	11
$CH_3 + O = CH_2O + H$	2.00 E + 12	-0.5	-0.3	11
$CH_3 + O_2 = CH_3O + O$	2.50 E + 9	-1.0	28.5	9

Table C-1. (Continued)

	A (cc, mole, sec)	N	E (kcal)	Ref.
REACTIONS DESCRIBING CH_4 OXIDATION MECHANISM (Cont.)				
$CH_3 + HO_2 = CH_4 + O_2$	1.00 E + 11	-0.5	6.0	8
$CH_3 + O_2 = CH_2O + HO$	3.00 E + 13	0.0	30.0	8
$CH_2 + O_2 = CH_2O + O$	5.00 E + 11	-0.5	7.0	8
$CHO + O = CO + HO$	3.00 E + 11	-1.0	0.5	10
$CH_2O + HO = CHO + H_2O$	1.00 E + 14	0.0	0.0	10
$CHO + HO = CO + H_2O$	3.00 E + 10	-1.0	0.0	10
$CH_2O + O = CHO + HO$	2.00 E + 11	-1.0	4.4	10
$CHO + H = CO + H_2$	3.00 E + 10	-1.0	0.0	10
$CH + O_2 = CHO + O$	5.00 E + 11	-0.5	6.0	8
$CH_2 + HO = CH + H_2O$	5.00 E + 11	-0.5	6.0	8
$CO + HO = CO_2 + H$	5.60 E + 11	0.0	1.08	10
$CO + O_2 = CO_2 + O$	1.00 E + 13	0.0	60.0	8
$CO + HO_2 = CHO + O_2$	3.00 E + 12	0.0	37.1	10
$HO_2 + H = O_2 + H_2$	2.50 E + 13	0.0	0.7	8
$HO_2 + HO = H_2O + O_2$	5.00 E + 13	0.0	0.0	8
$HO + HO = H_2O + O$	6.00 E + 12	0.0	1.0	8
$HO + H_2 = H + H_2O$	2.50 E + 13	0.0	5.2	8
$H + HO_2 = HO + HO$	2.50 E + 14	0.0	1.9	8
$HO + O = H + O_2$	2.50 E + 13	0.0	0.0	8
$H + HO = H_2 + O$	8.00 E + 9	-1.0	7.0	8
REACTIONS INVOLVING N, NO, N_2O, OR NO_2				
$N_2O + M = N_2 + O + M$	1.00 E + 14	0.0	50.0	8
$N_2 + M = N + N + M$	4.00 E + 21	1.6	225.0	8

Table C-1. (Continued)

REACTIONS INVOLVING N, NO, N_2O OR NO_2 (Cont.)

	A (cc, mole, sec)	N	E (kcal)	Ref.
$NO_2 + M = NO + O + M$	1.00 E + 16	0.0	65.0	8
$O_2 + N + M = NO_2 + M$	1.00 E + 19	1.0	0.0	9
$HO + N = H + NO$	6.00 E + 11	-0.5	8.0	10
$N + NO = N_2 + O$	3.10 E + 13	0.0	0.334	8
$N + O_2 = NO + O$	6.00 E + 9	-1.0	6.3	8
$NO + NO_2 = N_2O + O_2$	1.00 E + 12	0.0	60.0	8
$H + N_2O = HO + N_2$	8.00 E + 13	0.0	15.0	8
$N_2O + O = NO + NO$	1.00 E + 14	0.0	28.0	8
$N_2O + O = N_2 + O_2$	1.00 E + 14	0.0	28.0	8
$N + NO_2 = NO + NO$	4.00 E + 12	0.0	0.0	8
$N + NO_2 = N_2 + O_2$	1.00 E + 12	0.0	0.0	8
$NO + N_2O = NO_2 + N_2$	2.00 E + 12	0.0	40.0	9
$NO_2 + O = NO + O_2$	1.00 E + 13	0.0	1.0	8
$NO + HO_2 = NO_2 + HO$	5.00 E + 11	-0.5	3.52	9
$NO + HO = HO_2 + N$	5.00 E + 10	-0.5	96.5	9
$H + NO + M = HNO + M$	2.00 E + 16	0.0	0.0	9
$H + HNO = H_2 + NO$	1.00 E + 13	0.0	2.5	8
$HNO + NO = HO + N_2O$	2.00 E + 12	0.0	26.0	8
$HNO + HNO = N_2O + H_2O$	1.00 E + 10	-0.5	41.55	9
$HNO + O = HO + NO$	5.00 E + 11	-0.5	0.0	8
$HNO + HO = H_2O + NO$	1.00 E + 12	0.0	1.0	10

Table C-1. (Continued)

REACTIONS OF AMMONIA AND INTERMEDIATES	A (cc, mole, sec)	N	E (kcal)	Ref.
$NH_3 + O_2 = NH_2 + HO_2$	5.00 E + 11	-0.5	56.0	9
$NH_3 + O = NH_2 + HO$	8.20 E + 11	-0.5	0.0	9
$NH_3 + H = NH_2 + H_2$	1.90 E + 11	-0.67	3.4	9
$NH_3 + HO = NH_2 + H_2O$	4.00 E + 10	-0.68	1.1	9
$NH_2 + O_2 = NH + HO_2$	1.00 E + 13	0.0	50.5	9
$NH_2 + O = NH + HO$	9.20 E + 11	-0.5	0.0	9
$NH_2 + H = NH + H_2$	1.40 E + 11	-0.67	4.3	9
$NH_2 + HO = NH + H_2O$	3.00 E + 10	-0.68	1.3	9
$NH_2 + NO = N_2 + H_2O$	1.20 E + 10	0.0	0.0	9
$NH_2 + NH_2 = NH_3 + NH$	1.70 E + 11	-0.63	3.6	9
$NH + O = N + HO$	1.70 E + 10	-0.7	0.1	9
$NH + NO = N_2 + HO$	2.40 E + 12	0.0	0.0	9
$NH + H = N + H_2$	1.00 E + 12	-0.68	1.9	9
$NH + NH = N_2 + H_2$	3.60 E + 11	-0.55	1.9	9
$NH + HO = NO + H_2$	5.00 E + 11	-0.5	2.0	9
$NH + O = NO + H$	5.00 E + 11	-0.5	5.0	8
$NH + N = H + N_2$	6.00 E + 11	-0.5	0.0	8
$H + N_2O = H + NO$	1.00 E + 11	-0.5	30.0	8
$NH + HO = H_2O + N$	5.00 E + 11	-0.5	2.0	8
$H + HNO = NH + OH$	2.00 E + 11	-0.5	23.0	8
REACTIONS BETWEEN CARBON, HYDROGEN AND NITROGEN				
$CHN + N = CH + N_2$	5.00 E + 11	0.0	16.0	10
$CH_2 + N_2 = CHN + NH$	1.00 E + 14	0.0	55.0	10

Table C-1. (Concluded)

REACTIONS BETWEEN CARBON, HYDROGEN AND NITROGEN (Cont.)

	A (cc, mole, sec)	N	E (kcal)	Ref.
$CHO + N = CH + NO$	1.00 E + 14	0.0	48.6	10
$CHN + O = CH + NO$	1.00 E + 13	0.0	72.0	9
$CN + NH = CH + N_2$	1.00 E + 14	0.0	40.0	10
$CN + NO = CO + N_2$	3.00 E + 11	0.0	0.0	8
$CN + O_2 = CO + NO$	3.00 E + 11	0.0	0.0	8
$CN + O = CO + N$	5.00 E + 11	-0.5	9.63	9
$CHN + OH = CN + H_2O$	2.00 E + 11	-0.6	5.0	8
$CO_2 + N = CO + NO$	2.00 E + 11	-0.5	25.0	8
$CH_2O + NO = HNO + CHO$	5.00 E + 11	-0.5	27.0	9
$CH_3O + NO = HNO + CH_2O$	5.00 E + 11	-0.5	4.23	9
$CO + HNO = CO_2 + NH$	5.00 E + 8	-0.5	7.0	9
$CH_3 + HNO = CH_4 + NO$	5.00 E + 11	-0.5	0.0	8
$CHO + NO = CO + HNO$	2.00 E + 11	-0.5	2.0	8

where the units are note, cm^3, sec, ^oK and kcal. The values of the constants used originally, A, N, and E, were those listed by Engleman(8) or estimated by the method of Tunder, et al(9). A recent report by Benson, et al(10) lists estimated Arrhenius parameters for several of the reactions included in the synthesized set. All of the calculations carried out used the rates given in Table C-1, all of which are within the estimates given by Benson, et al(10). No attempt was made to screen the reaction set.

C.4 EVALUATION OF REACTION SET AGAINST STIRRED REACTOR DATA

Having assembled a reaction set which seemingly included all the key reactions reported in the literature concerning NO formation and destruction, the reaction set was used in the KAP program in the perfectly stirred reactor mode, and an attempt was made to calculate the stirred reactor data reported by Bartok, et al(6). This data had been used previously by Waldman et al(11) for CH_4-O_2-N_2 mixtures. The experimental investigation also included the addition of NH_3 and NO to the stirred reactor. A comparison between the measured and predicted NO concentrations is presented in Figures C-1, -2 and -3. The stirred reactor calculations were carried out with a heat loss of 0.028/sec^oK (see reference 11 for further discussion).

The 33 reaction set proposed by Waldman et al(11) was tested with the methane/air stirred reactor data with the stated heat loss and found to be unsatisfactory. Predicted NO concentrations were almost one order of magnitude below the experimental data. Also, for equivalence ratios greater than 1.33 the calculated NO concentrations were independent of equivalence ratio. The mechanism was inadequate because it did not include reactions of the Path B type which allow the formation of N_2 from XN intermediates.

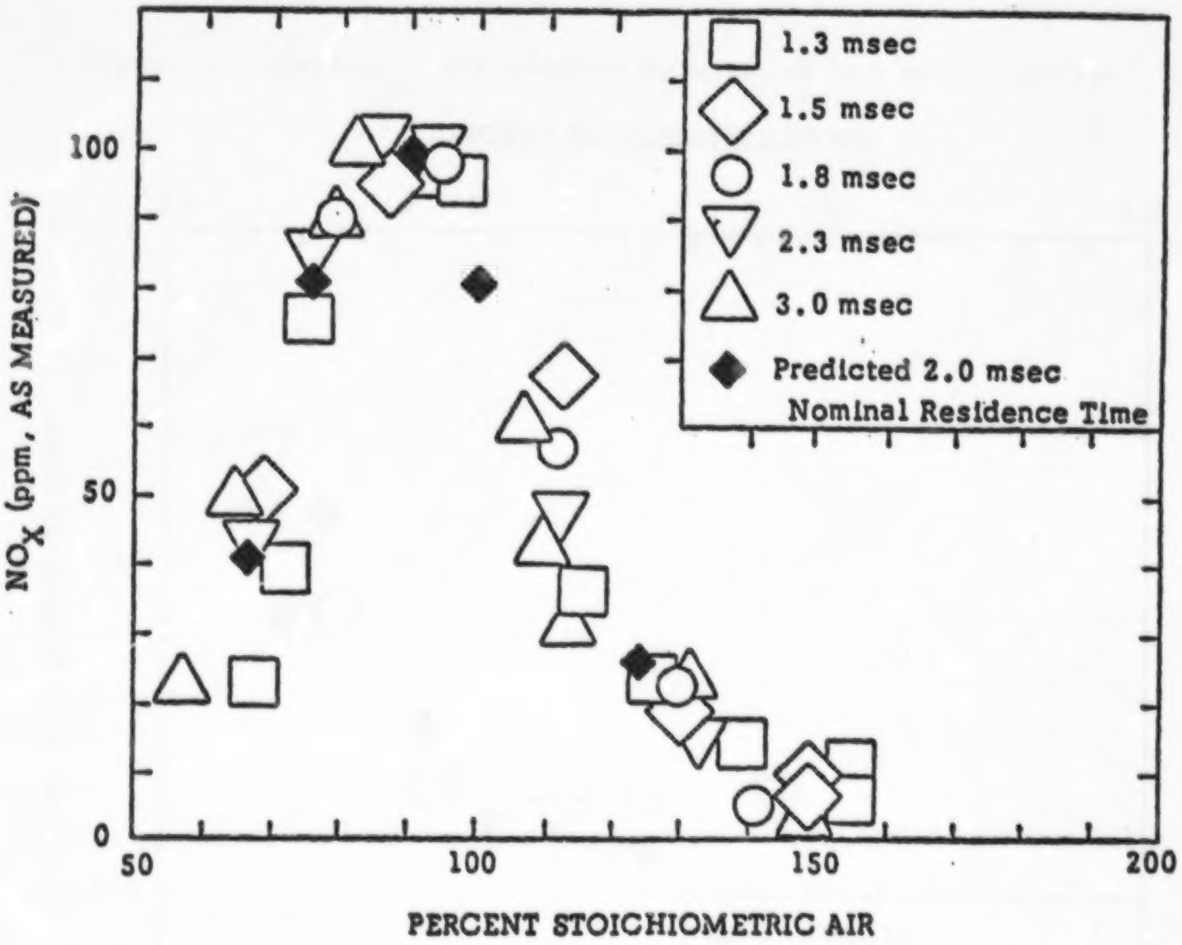

Figure C-1. Comparison of Measured(6) and Predicted NO_x Concentration at the Exit of a Stirred Reactor

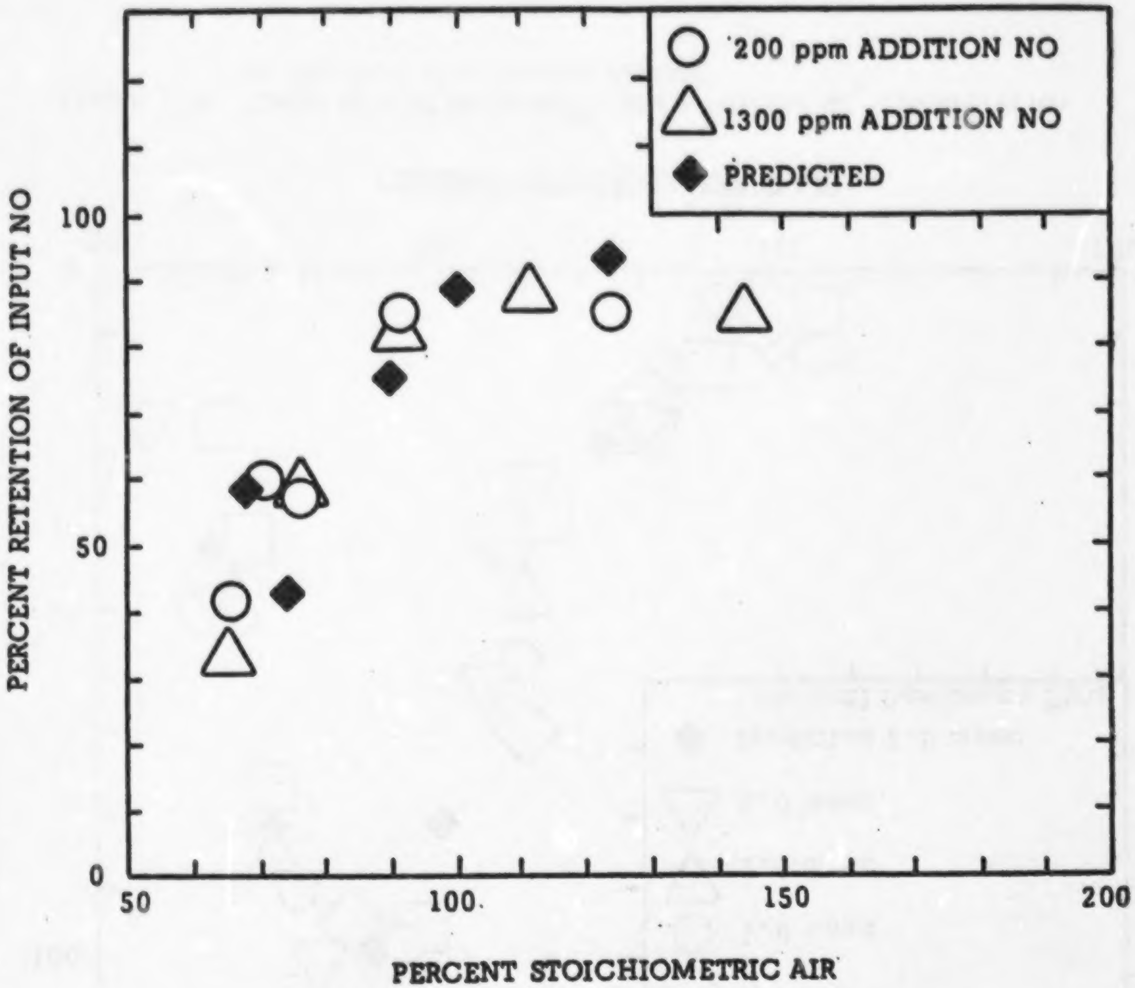

Figure C-2. Measured$^{(6)}$ and Predicted NO Retention in a Stirred Reactor

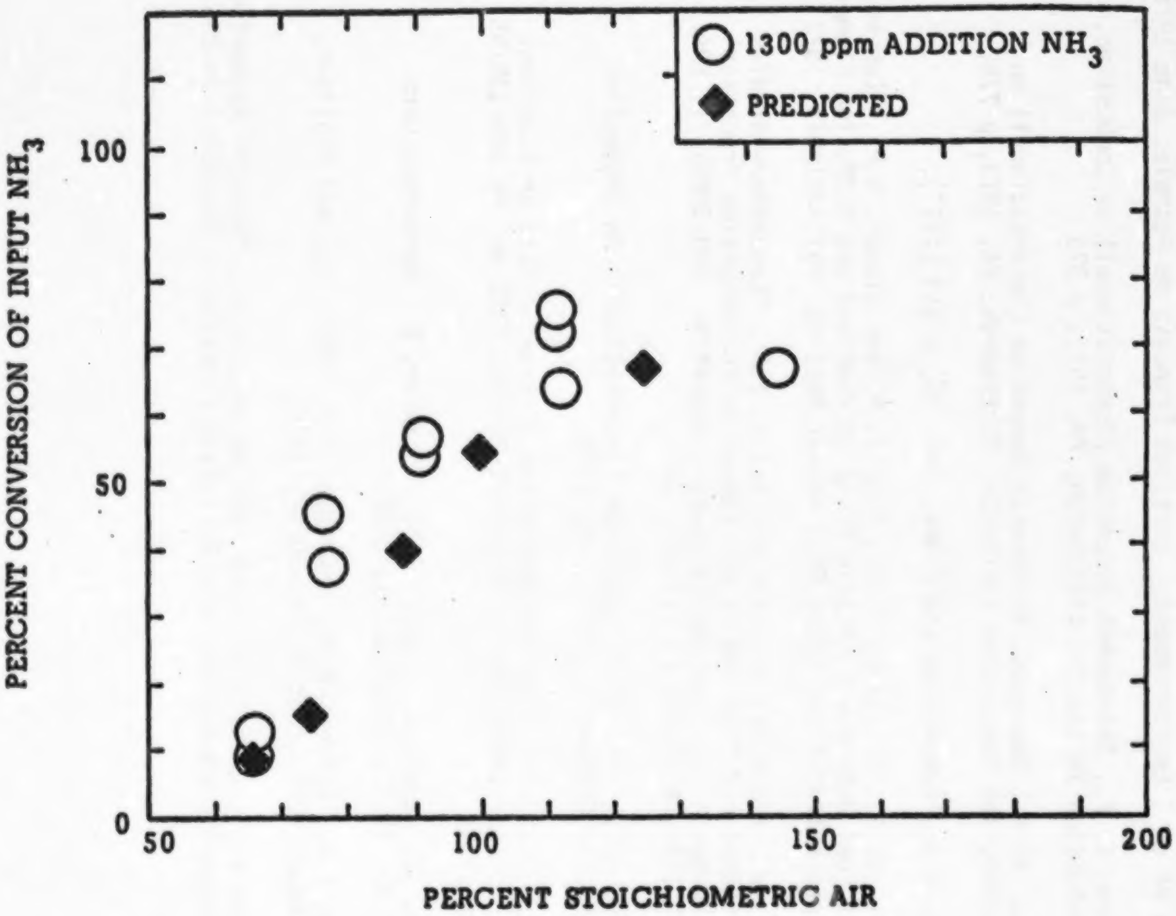

Figure C-3. Measured(6) and Predicted Conversion of NH_3 to NO_x in a Stirred Reactor

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